SIMTRA - User Manual

version 2.1.1

Research Group DRAFT

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Contents

1 About

SIMTRA is a test particle Monte Carlo code developed to simulate the metal flux during magnetron sputtering. Using predefined surfaces the user can create a geometrical representation of his or her experimental setup which is visualized by the graphical user interface. The movement of a number of particles, generated with initial conditions (position, energy and direction) from a target surface, is tracked until they cross one of the defined surfaces. Several options are available to customize the particle generation and transport through the gas phase such as: custom racetracks, initial energy and angular distributions, in- or exclude gas motion and diffusion and several interaction potentials.

2 Requirements

SIMTRA is compiled to run on a Windows platform targeting .net 4.5 framework. In case of issues with the 3D visualisation, you might need to update the openGL drivers of your graphics card.

To run an actual simulation, the only extra input data besides the configuration that is to be provided by the user is an adequate description of the racetrack (see section 8). The user can choose to use an initial angular and energy distribution from SRIM (see section 9), in which case of course a corresponding SRIM output file should be available as well.

3 Reference

When using this software for publications, please use the following reference:

The metal flux from a rotating cylindrical magnetron: a Monte Carlo simulation. K. Van Aeken, S. Mahieu, D. Depla, *Journal of Physics D.: Applied Physics* 41 (2008) 205307

For application examples, check out the following overview article:

Magnetron sputter deposition as visualized by Monte Carlo modeling. D. Depla, W.P. Leroy, *Thin Solid Films 520 (2012) 6337*

4 Current version

The latest stable version is `v_2.1.1`. All changes of future releases will be listed in the file `releasenotes.txt`, together with known issues and whether or not any of the implemented features still need additional testing. Both the code as well as this manual should be considered as work-in-progress. Please read the disclaimer, as it applies to all SIMTRA releases. Any bugs, crashes or suggestions can be reported to ✉ francis.boydens@ugent.be.

5 Installation and start-up

Download and unpack the `.rar` file. Double click the `.exe` file inside the unpacked folder and you're good to go. Besides the `.exe` file, the uncompressed SIMTRA folder contains the following subfolders and files:

- 🗀 `Examples`: a folder with some example input and output files
- 🗀 `NascentAngular`: contains several user defined initial angular distributions (see section 9)
- 🗀 `outputdata`: an optional folder to save output data
- 🗀 `RacetracksCylinder`: contains racetrack data of several rotatable targets used at DRAFT
- 🗀 `RacetracksPlane`: contains the racetrack data of a standard circular planar magnetron used at DRAFT
- 🗀 `ScatteringAngleTables`: a folder containing the data for the different interaction potentials
- 🗀 `SputterFiles`: a folder containing an example of an SRIM output file that can be used for the initial energy and/or angular distribution.
- 🗎 `_recentfiles.xml`: an xml file used to generate the most recently used files in the GUI menu.
- 🗎 `user_manual_v_X.Y.Z.pdf`: a copy of this file.

- releasenotes.txt: a text file updated with each release, listing any new features, bug fixes and known issues.

Of all folders and files listed above, only ScatteringAngleTables should not be moved nor deleted.

6 SIMTRA basics and quick start

6.1 Single simulation runs

In the following section, the basics of a SIMTRA simulation will be introduced by configuring a simple setup. A 5×5 cm^2 substrate is placed 15 cm away from an aluminum target, mounted on a planar magnetron. The target is sputtered in an argon atmosphere of 0.5 Pa at room temperature. We want to obtain the deposition profile on the substrate. A SIMTRA configuration consists of three parts:

1. a vacuumchamber, defining the outer boundaries for the sputtered particles
2. a magnetron object, containing a target which determines the starting position of the particles
3. any number of other 'dummy' objects on which the particles can be deposited, in this case on single square substrate surface

6.1.1 The vacuum chamber

In the main window menu, click Object » New » Vacuum chamber. This opens the Chamber Design window (Fig. 1). Select the shape of the chamber (cuboid or cylinder), fill out the dimensions, click the button below the dimensions to select the sputter gas, enter the gas pressure and gas temperature. In case you are interested in the deposition profile on the chamber walls, check the *save deposition on chamber walls* box and enter the grid size for each dimension. If you want specific info on each particle that is deposited on the any of the chamber walls, check the box *save individual data*. For more info on data collection and output data in general, see section 11. Click *Add chamber* to add the chamber to the configuration. The Chamber Design window closes and you're back at the main window. The chamber is drawn in the visualization window.

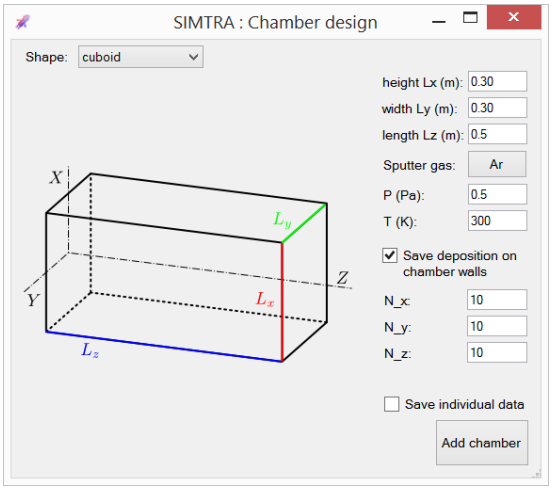


Figure 1: The Chamber Design window.

6.1.2 The magnetron

Again in the main window menu, click Object > New > Magnetron. The Object Designer main window opens in magnetron mode with three subwindows: the geometry window, the visualization window and the target and transport settings. A custom object geometry can be defined by adding any number of surfaces and setting their dimensions and orientation (see section 7). For now we will use a template of a planar magnetron. In the designer main menu, click Geometry > Template > Magnetron > Planar. The planar magnetron template window opens, enter a name for the object and edit the dimensions as you wish. Click *Create object* to generate the necessary surfaces. Six different surfaces are now listed in the geometry window (Fig. 2). By selecting any of them, you can inspect their position, orientation and dimensions. The selected surface is highlighted in blue in the visualization window. For a more detailed description of object design, see section 7.

For now, let's inspect the surface corresponding to the target (no. 6) by selecting it. Notice that the target is positioned at $z = 0.0217\ m$ from the object center. This will be important for correctly setting the target-substrate distance later on.

Next, the following input has to be configured in the *Target & transport settings* window (Fig. 3):

- Set a target element by clicking the button and selecting it.
- Enter the number of particles that should be simulated

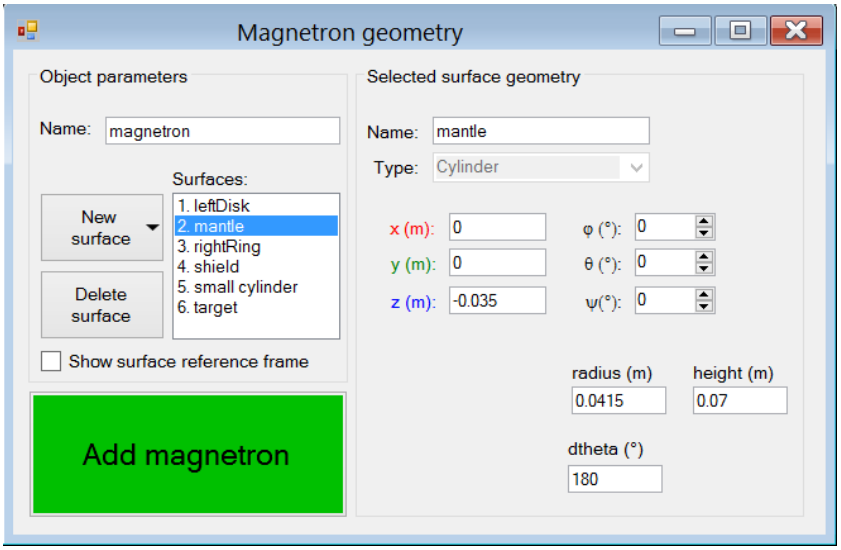


Figure 2: The magnetron geometry window listing the six surfaces of a predefined planar magnetron.

- Enter the number of the surface from the list in the geometry window that corresponds to the target surface. (In this case, this is surface number 6)

- Enter or browse to the file containing the racetrack data. For now we will use `RacetracksPlane/racetrackGent.txt`. For more info on racetrack files, see section 8.

- Set the corresponding racetrack type. In this case it's an axial symmetric racetrack file. Again, for more info on racetrack files and types, see section 8.

- Select which initial angular distribution you wish to use. For a simple cosine distribution, select *User*, set $c1 = 1$ and the other coefficients to 0. If you wish to use an angular distribution obtained with SRIM, you will be asked to browse to the SRIM output file.

- Select the initial energy distribution: either a Thompson distribution or from an SRIM simulation. By default, the surface binding energy is taken to be equal to the sublimation energy of the target element, but can be edited as you wish. In case of a Thompson distribution, the maximum ion energy has to be given as well.

- Check or uncheck the boxes *With gas motion* and *Go to diffusion* depending on whether or not these should be taken into account. Note that when *Go to diffusion* is unchecked, the computation time increases significantly. For now leave both boxes checked. For more info on the transport description see section 10.

- Select the interaction potential. Use a screened Moliere for now or see section 10 for more info.

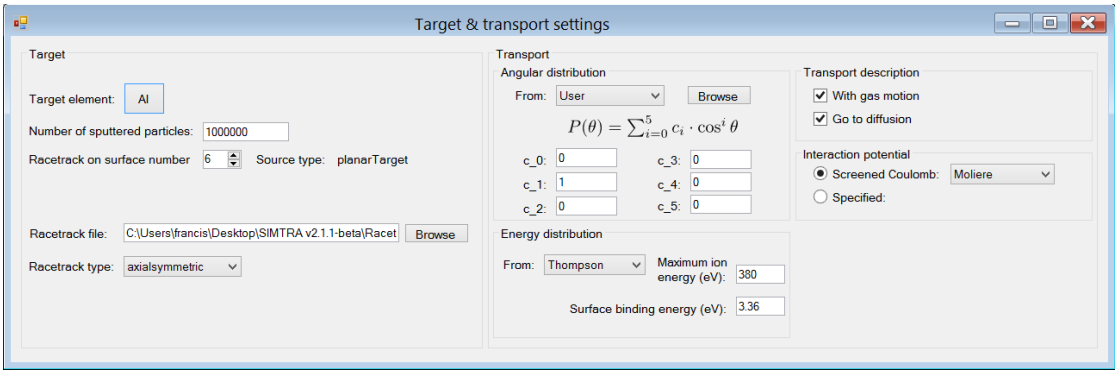


Figure 3: The Chamber Design window.

Geometry, target and transport settings are now configured. Click *Add magnetron* to add the magnetron to the setup and close the Designer window.

Back in the main window, the magnetron is now listed together with the vacuum chamber in the *Object configuration* window (Fig. 4) and is drawn in the visualization window. Each object listed here can be hidden or shown by (un)checking the box next to its name. The position and orientation of any object can be set by selecting it and setting the (x, y, z) coordinates of its origin and adjusting the Euler angles ϕ, θ and ψ[1]. By checking the box *Show object reference frame*, the local reference frame of the object is drawn using dashed lines.

Below the list of the objects, a list of surfaces of the selected object is given. Similar to the list of objects, each individual surface can be hidden or shown by (un)checking it[2]. The data collection options of each individual surface can be set by selecting it and checking the appropriate boxes (see section section 11). For now, we are only interested in redeposition on the target, so select the target surface (no. 6), check the box *Save averaged data* and enter a grid size.

In the *Overview* window, a summary is given of the most important settings for the simulation, i.e. chamber configuration and target and transport settings. Sputter gas, pressure, temperature, target element and number of simulated particles can be changed directly in the overview window. Clicking any of the other buttons will either open the Chamber or Object Design window to edit the respective property.

[1] These correspond to an active rotation around the Z, Y' and Z'' axes resp.
[2] Unchecking an object or a surface *does not* exclude it from the simulation!

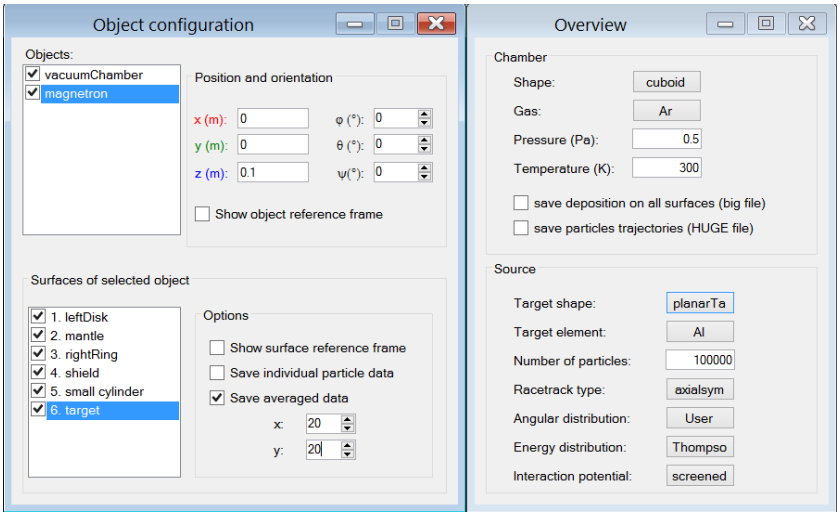


Figure 4: The Object Configuration and Overview windows.

6.1.3 Adding a dummy object

With chamber and magnetron defined, only a substrate is still missing. This will be a dummy object consisting of a single surface. In the main window, click Object › New › Dummy object. Similar to adding a magnetron, the Designer window will open, with only two subwindows now. In the *Object Geometry* window, enter a name for the substrate object. Click New surface › Rectangle and enter the dimensions of the substrate. Note: *dx* and *dy* are *half* the length and width of the rectangle, so for a substrate of 5×5 cm^2, enter twice the value 0.025 (Fig. 5). Click *Add dummy object* to add the substrate to the setup and close the Designer.

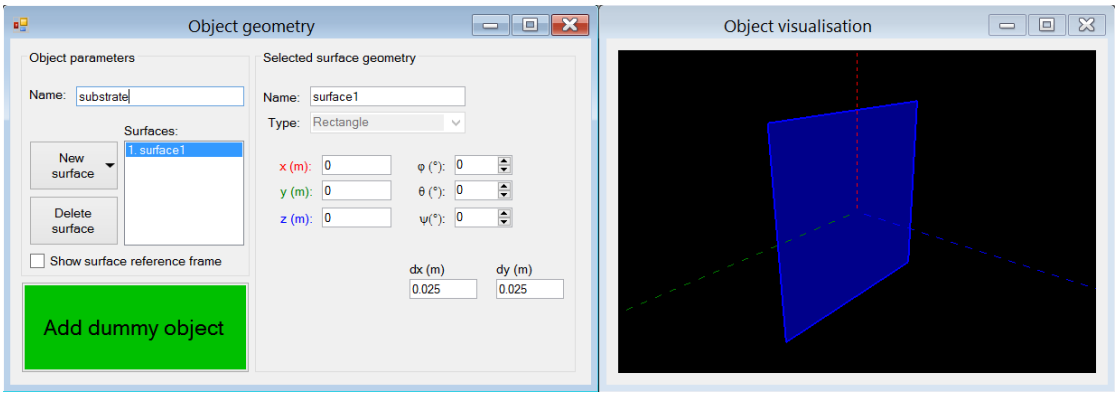


Figure 5: Defining a rectangular substrate of 5×5 cm^2.

Back in the main window, the substrate is listed together with the chamber and the magnetron. As seen in the visualization window, the substrate is currently positioned

in the origin, so it still needs to be moved to the correct location. Recall that we put the magnetron at $z = 0.10\ m$ and that the target surface was at $z = 0.0217\ m$ from the magnetron center. Hence, assuming we want to simulate a target-substrate distance of 15 cm, we need to move the substrate to $z = 0.10 + 0.0217 + 0.15 = 0.2717\ m$ (Fig. 6). To set the data collection for the substrate, select surface1 from the list of surfaces, check the box *Save averaged data* and enter a grid size. As we defined a substrate of 5×5 cm^2, entering twice the value 5, will divide the substrate in cells of 1×1 cm^2, where each arriving particle will be collected.

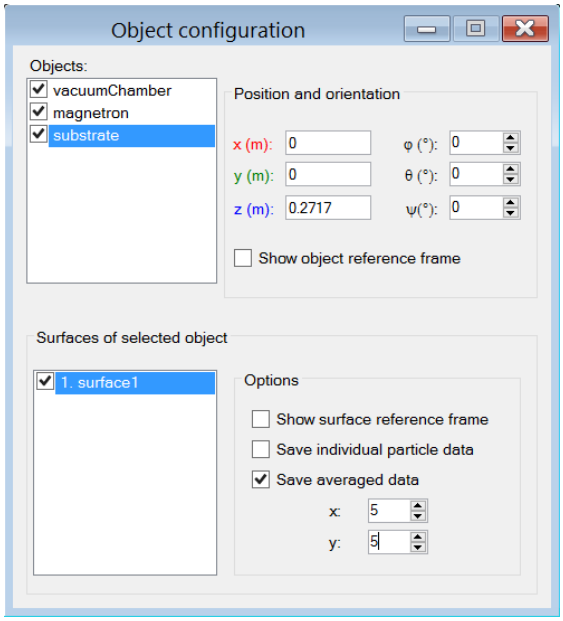


Figure 6: Defining a rectangular substrate of 5×5 cm^2.

6.1.4 Run the simulation

Run the simulation either by clicking Simulation › Start current, pressing the green 'play' arrow, or using the hotkey combo Ctrl + r. If you have not saved the input file before, you will be prompted to save the inputfile. Let's name it `my_first_simtra_sim` and save it in the folder `C:▸...▸SIMTRA_vX.Y.Z▸outputdata`. Hitting ok will save the input file and start the simulation. A progress bar indicates the progress of the current simulation. A simulation can be canceled at any time by pressing the red stop button or by Simulation › Cancel current. Note that no data is saved until all particles have been simulated, so no intermediate results are written to disk[3].

By default, the outputdata is saved in sub folder of the parent directory of the input

[3] this might change in a future release.

file. The subfolder has the same name as the input file. In this case all output files are located in C:▸...▸SIMTRA_vX.Y.Z▸outputdata▸my_first_simtra_sim. This default behavior can be overridden by specifically entering an output folder in the *output folder* field of the Main window, next to the cancel button.

6.1.5 Check output

The deposition profile of the substrate can be found in the file

substrate_surface1_surfaceNr1_N.txt

which is saved in the folder outputdata▸my_first_simtra_sim▸depositionExtraObjects.

This file contains 5 rows and 5 columns, corresponding to the grid defined in the *Object configuration* window (Fig. 7). For more info on the output data, see section 11

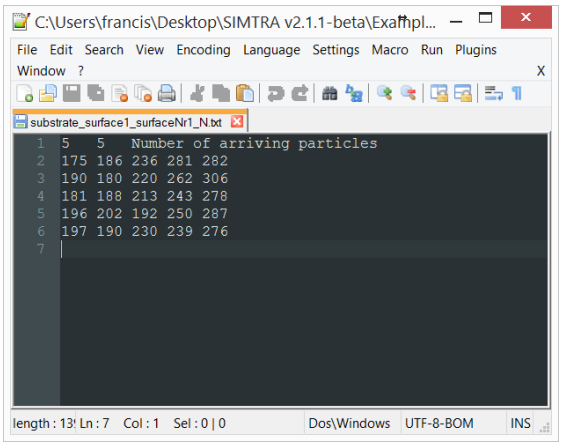


Figure 7: Example of an output file containing the total number of particles that have arrived in each cell of the substrate.

6.2 Batchrun mode

The GUI also allows to batch process multiple .sin files. To do so, create each input file as described above and save them. Next, go to Simulation ⟩ Start multiple. This will open the batchrun window (Fig. 8). Any number of input files can be added to the list by either Add ⟩ files or Add ⟩ folder. The latter will load all .sin files found in the selected

folder into the list[4]. Queued files are listed in blue, successfully completed input files in green, the current input file in orange, and input files for which one or more errors have occurred in red. Hitting view runlog will give a detailed overview of all simulation runs.

`Examples ▸ Example2_batchrun` contains four input files with the same configuration, only different target elements. These can be used to illustrate the use of this run mode.

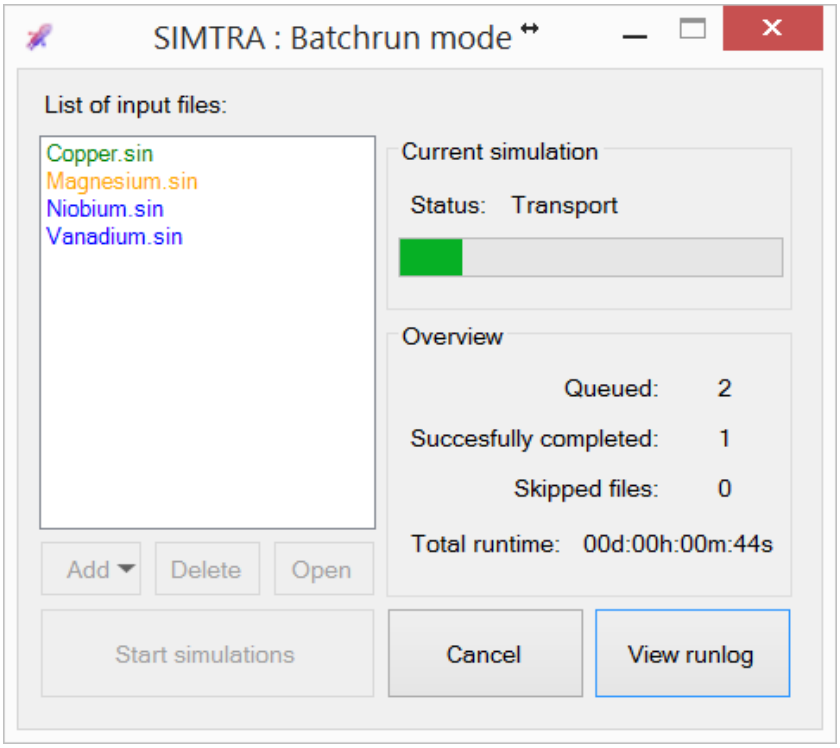


Figure 8: The batchrun window.

7 Object design

7.1 Reference frames

SIMTRA uses three different type of reference frames. (X,Y,Z) axes are always drawn in the resp. colors red, green, blue. Figure 9 shows an example of the reference frames:

- a global reference frame (full lines). Object positions and orientations which are set in the main window are always defined in this global reference frame.

[4]Note that only the filenames are listed, not their full path, so it's possible that the same name might occur twice in this list, this won't give any errors

- an object reference frame (dashed lines): Each object has its own local reference frame. Positions and orientations of the object surfaces are always defined with respect to this reference frame.

- a surface reference frame (dotted lines): each surface in turn has its own reference frame as well. When a particle hits a surface, its local coordinates with respect to the surface reference frame are calculated. The grid (N_1, N_2) for the average particle data is defined in the local surface reference frame (see section 11).

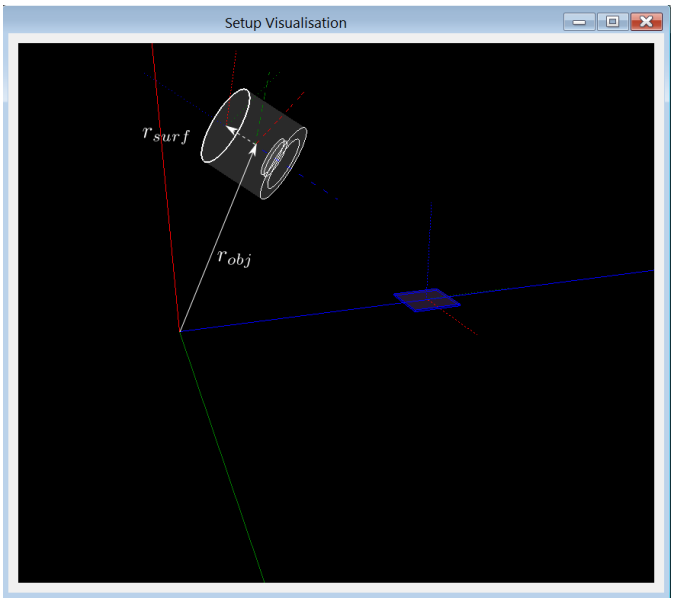


Figure 9: Illustration of the different reference frames: the position of the object r_{obj} is defined in the global reference frame. The position of the circular backside of the magnetron r_{surf} is defined in the reference frame of the magnetron (dashed lines).

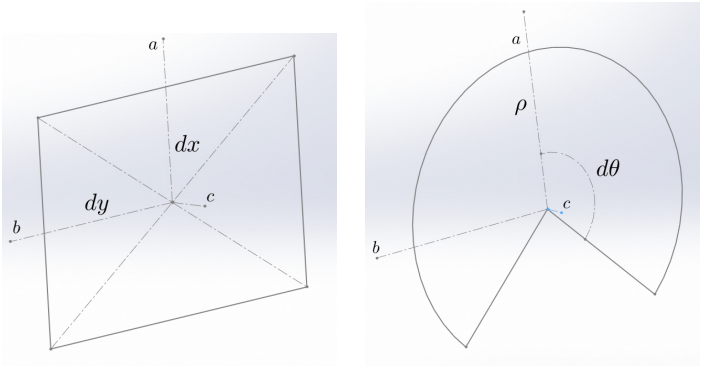
The orientation of a reference frame is set by the Euler angles (ϕ, θ, ψ) for the intrinsic rotations around the axes (Z, Y', Z'').

7.2 Surface types

Each simtra object consists of one or more surfaces, which are defined by a surface origin, orientation and a set of parameters. Several types of surfaces are available: planar surfaces (rectangular and circular, with or without a central opening), cylindrical surfaces, conical surfaces (truncated or not) and spherical surfaces. Depending on the surface type, different parameters need to be provided by the user:

surface type	parameter	description
rectangular	dx, dy	half (!) the length and width of the rectangle along the local axes a and b
circular	radius, $d\theta$	radius (in meters) and range of the central angle of the circle segment in degrees ($\theta = -d\theta, ..., d\theta$, so 180 for full circle)
cylindrical	radius	radius of the cylinder
	length	cylinder length in meters
	$d\theta$	range of the opening angle of the cylinder in degrees ($\theta = -d\theta \cdots + d\theta$, so 180 for full cylinder)
conical	ρ	radius of the small/large circle
	height	height of the cone
	dθ	range of the opening angle of the cone in degrees ($\theta = -d\theta \cdots + d\theta$, so 180 for closed cone)
spherical	$d\theta$, $d\phi$	range of resp. polar and azimuthal angles θ and ϕ, with $\theta = 0, ..., d\theta$ and $\phi = -d\phi, ..., d\phi$

Table 1: Description of the surface parameters for the different surface types.



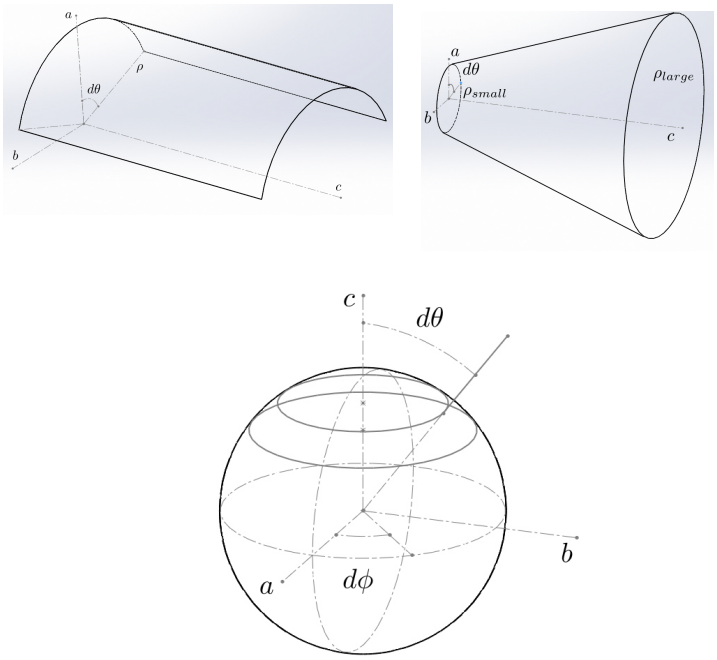


Figure 12: Different surface types.

8 The racetrack

The racetrack file is used to create a probability function for the initial position of the simulated particles. Three different formats for the file can be used: axialsymmetric, profilometry, rotatable.

Note that the racetrack file is only used to sample an initial position of the simulated particle. The shape or depth is not taken into account during the simulation of the transport, as a completely flat target surface is assumed.

8.1 Axialsymmetric

As the name implies, this assumes an axial symmetric racetrack and is mostly used when simulating planar circular targets. The file that is provided should contain two columns. First column is the radial distance from the target center in meter (!), second column the measured racetrack depth. The unit of the second column is of no importance as it is normalized when calculating the probability function.

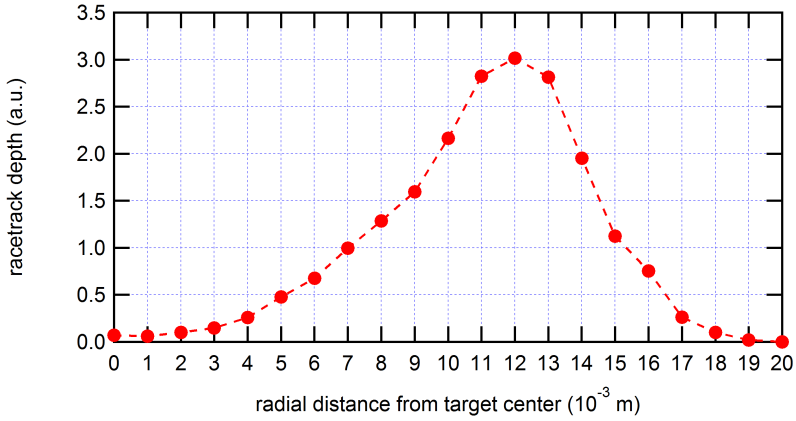


Figure 13: Example of a racetrack file in case of an axial symmetric racetrack.

8.2 Profilometry

A file containing an M x N matrix should be provided where each value is the depth measured at position (col_index,row_index). It is assumed that the center of the file coincides with the center of the target surface. col_index determines the position along the local a axis of the surface, row_index the position along the local b axis.

9 Initial angular and energy distributions

Two options are available for the initial energy distribution. It is either taken from an SRIM file or from the analytical Thompson distribution. In case of the latter the maximum energy of the incident ions has to be given as well.

For the angular distribution an SRIM output file can be used as well, or the user can give the coefficients c_i of a custom distribution:

$$f(\cos\theta) = \sum_{i=0}^{5} c_i \cdot (\cos\theta)^i \tag{1}$$

Note that when using an SRIM file for either the initial angular or energy distribution, the file should contain a large amount of simulated particles since energy and emission angles will be sampled randomly from the list.

10 Transport description

Coming soon.

11 Data collection and output files

Once the simulation has successfully finished, the following files and subfolders can be found in the output folder:

- `depositionChamber`: is present only in case any of the boxes *Save deposition on chamber walls* or *Save individual data* were checked and contains the averaged and/or individual data files for each chamber wall.
- `depositionDummyObjects`: contains the deposition data on any of the dummy objects
- `depositiongraph`: can be ignored.
- `depositionMagnetron`: contains deposition data on all surfaces of the magnetron object
- `errors.txt`: an overview of any errors that might have occurred during the simulation run.
- `initialAngularDistribution.txt`: a histogram of the cosine of the emission angles of all simulated particles
- `initialEnergyDistribution.txt`: a histogram of the initial energy of the particles.
- `*.sin`: the input file of the simulation. A `.sin` file contains all info required to run a simulation and can be opened with the GUI through File > Open or Ctrl + o
- `specificInformation.txt`: a file containing the run time and date of the simulation, the total number of particles that were redeposited onto the target and the particle diffusion length.

For each defined surface two options are available:

1. Save averaged particle data

2. Save individual particle data

and can be set by selecting the specific surface in the *Object geometry* subwindow of the main window and checking the appropriate boxes.

Output files for each surface can be found in the folder:

`outputfolder‣depositionXXX‣object_name‣surface_name`

where XXX is either Chamber, DummyObjects or Magnetron, depending on the type of object the surface belongs to.

11.1 Average particle data

When *average particle data* is checked, a grid of size $N_1 \times N_2$ will be defined on the surface and the average data of particles arriving in each cell will be calculated. Depending on the surface type different surface parameters will be subdivided by N_1 and N_2 to obtain a homogeneous grid. See Table 2 for an overview.

surface type	N_1	N_2
planar	a	b
cylindrical	θ	c
conical	θ	c^2
spherical	$\cos\theta$	ϕ

Table 2: Overview of surface parameters/dimensions that are subdivided by N_1 and N_2.

The following output files are generated:

- `E.txt`: average particle energy (eV)
- `Flight.txt`: the average time between particle emission and deposition (s)
- `Ksi.txt`: average cosine of the angle of incidence with respect to the surface normal
- `N.txt`: total number of particles that have been deposited per surface cell
- `Ncoll.txt`: average number of collisions the particles have undergone

- `Path.txt`: the average distance the particles have traveled between emission and deposition
- `ScatAngle.txt`: the average scattering angle of the particles

The same terminology is used for the surfaces of the vacuum chamber in case *save average data* was check in the *Chamber design* window, with the exception that the names of the chamber walls are automatically generated based on their position. E.g. the files in directory `depositionChamber/xmax` contain the data for the top wall of the chamber.

11.2 Individual particle data

The option *Save individual particle data* saves the data listed in Table 3 of each single particle that is deposited on the surface in

`IndividualData.txt`

header name	description
particle no.	the number of the test particle
startpos_(x,y,z)	global (x,y,z) coordinates of the initial position of the particle
pos_(x,y,z)	global (x,y,z) coordinates of where the particle was deposited
local_(1,2,3)	position where particle was deposited in local surface coordinates
nvec_(x,y,z)	vector of incidence on the surface in the global reference frame
nvec_(a,b,c)	vector of incidence in the local reference frame of the surface
E	energy of the particle when it was deposited
coll	number of collision between emission and deposition
path	total distance the particle has travelled (m)
total scat angle	total scattering angle of the particle (rad)
flight time	the time the particle spent in the gas phase (s)

Table 3: Data saved when *Save individual particle data* option is checked.

12 FAQ

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