Report CLRP-08-01
Manual of `backscatter_clrp`:
An EGSnrc user-code for backscatter calculations

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February 22, 2008

1 Introduction

This report is intended for those in any applied physics field in which charged particle backscatter calculations are of interest - e.g., analytical surface science, scanning electron microscopy, electron and positron probe microanalysis and medical physics.

In two recent papers,[1,2] an exhaustive study of the capabilites and limitations of the EGSnrc[3,4] Monte Carlo radiation transport code in backscatter calculations have been investigated. As a by-product of the study, a new EGSnrc user-code, `backscatter_clrp`, dedicated for backscatter calculations, was developed. The user-code `backscatter_clrp` can calculate the backscatter coefficient, the energy spectra and the angular distributions of backscattered charged particles. The goal of this report is to describe `backscatter_clrp` and to provide instructions on how to use it for backscatter calculations.

2 Definitions

Figure 1 and table 1 define the backscatter parameters used in the user-code `backscatter_clrp`, in the related publications and throughout this report. Fig 1 Table 1

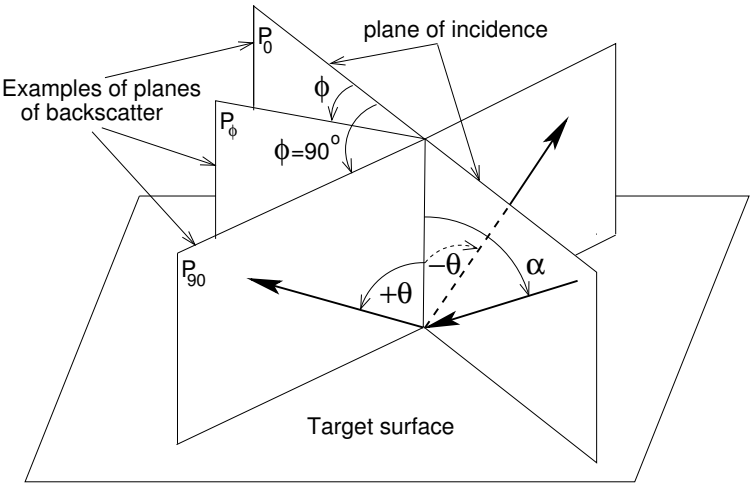

Figure 1: Definition of angles and planes used in the user-code backscatter_clrp and throughout this report (reproduced with modifications from Ali and Rogers[2]).

3 Initial setup

• Install the EGSnrc system. The EGSnrc installation package is available at http://www.irs.inms.nrc.ca/EGSnrc/EGSnrc.html.

• Download the file backscatter_clrp.tar to the EGSnrc home directory, i.e. to $EGS_HOME. The file is available at http://www.physics.carleton.ca/clrp/backscatter and it contains the full package of the user-code backscatter_clrp.

• Extract the files of the package using the Unix command tar -xf backscatter_clrp.tar or any other extracting utility. Extracting the files will create a new directory $EGS_HOME/backscatter_clrp and there should be 10 files in it. These 10 files are: the source code (backscatter_clrp.mortran), three files necessary for compilation (Makefile, backscatter_clrp.make and backscatter_clrp.io), two sample input files (sample_input_01.egsinp and sample_input_02.egsinp), one sample cross section data file (backscatter_clrp.pegs4dat), the two papers presenting the backscatter study (Ali_Rogers_PMB.pdf and Ali_Rogers_JPhysD.pdf) and this report (CLRP-08-01.pdf).

• Move the sample cross section data file from $EGS_HOME/backscatter_clrp to one of the two existing directories $EGS_HOME/pegs4/data or $HEN_HOUSE/pegs4/data.

• Compile the user-code by typing make. Now an executable version of the user-code should exist in $EGS_HOME/bin/g77, $EGS_HOME/bin/ifort or something similar, depending on the FORTRAN compiler used. Whenever changes are made to the source code or to the two make files, the user-code needs to be re-compiled for the changes to take effect.

• To run the user-code, type ex backscatter_clrp file1 file2, where file1.egsinp and file2.pegs4dat are the names of the input file (e.g., sample_input_01.egsinp) and the cross section data file (e.g., backscatter_clrp.pegs4dat), respectively. The contents of the two types of files are discussed below. Note that the command to run the user-code does not include the extensions .egsinp and .pegs4dat.

Table 1: Definition of the parameters used in the user-code backscatter_clrp and throughout this report.

parameter (units)	definition
E_0 (keV)	Kinetic energy of the incident charged particle beam.
E (keV)	Kinetic energy of the backscattered charged particle.
P_0	Incidence plane: a plane defined by the vector of the incident beam and the vector normal to the target surface.
P_ϕ	Backscatter plane: a plane defined by the vector of the backscattered charged particle and the vector normal to the target surface.
ϕ (degrees)	Plane angle: angle between the backscatter plane and the incidence plane. $0 \leq \phi \leq 90$.
α (degrees)	Incidence angle: angle between the vector of the incident beam and the vector normal to the target surface. $0 \leq \alpha < 90$.
θ (degrees)	Backscatter angle: angle between the vector of the backscattered charged particle and the vector normal to the target surface. θ is positive in the forward half of P_ϕ and negative in the backward half. $-90 < \theta < 90$.
$\Delta\Omega$ (sr)	Solid angle subtended by the detector. $\Delta\Omega = 2\pi$ sr if the detector is a hemispherical collector. $0 < \Delta\Omega \leq 2\pi$.
$d^2\eta(P_\phi, E, \theta)/dE\ d\Omega$ (keV^{-1} sr^{-1})	Local energy spectrum: number of charged particles backscattered in a given plane, P_ϕ, with energy between E and $E + dE$, at a backscatter angle between θ and $\theta + d\theta$, per unit energy, per unit solid angle, per incident charged particle.
$d\eta(E)/dE$ (keV^{-1})	Overall energy spectrum: number of charged particles backscattered in the hemisphere above the target surface, with energy between E and $E + dE$, per unit energy, per incident charged particle.
$d\eta(P_\phi, \theta)/d\Omega$ (sr^{-1})	Angular distribution: number of charged particles backscattered in a given plane, P_ϕ, at a backscatter angle between θ and $\theta + d\theta$, per unit solid angle, per incident charged particle.
η_- (η_+) (%)	Electron (positron) backscatter coefficient: the probability that a charged particle incident on a semi-infinite target backscatters into the hemisphere above the target.

4 Cross section data

Running any EGSnrc user-code requires a cross section data file with an extension `.pegs4dat` located either in `$EGS_HOME/pegs4/data` or `$HEN_HOUSE/pegs4/data`. For user convenience, the file `backscatter_clrp.pegs4dat` is included in the package of the user-code. The sample cross section data file includes data for electrons, positrons and photons in the energy range of 1 keV to 2 MeV with Rayleigh scattering and density effects[5] included. The elements included are: Be, C, Na, Mg, Al, Si, Ti, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ge, Mo, Rh, Ag, Sn, W, Re, Pt, Au, Pb and U. The user can also generate additional data for other elements, mixtures and compounds using the graphic user-interface `egs_gui`[4] by typing `egs_gui` then clicking on `PEGS Data` when the GUI is launched. Any newly-generated dataset can either be saved in a new `.pegs4dat` file or appended to an existing one. Also, there are a few cross section data files that are included in the standard EGSnrc package and they are located in `$HEN_HOUSE/pegs4/data`. To find the names of the media included in a particular data file (`backscatter_clrp.pegs4dat` for example), the user can use the Unix command `grep` as follows: `grep 'MEDIUM' backscatter_clrp.pegs4dat`.

CAUTION: Because of positron/electron annihilation, when an incident *positron* beam with kinetic energy E_0 (in keV) is simulated, the `.pegs4dat` file must contain electron/positron data up to at least E_0 + 2×511 keV, and photon data up to at least E_0 + 511 keV. For example, the data in `backscatter_clrp.pegs4dat`, which is generated up to 2 MeV, support an incident positron beam of kinetic energy no greater than 2000 - 2×511 = 978 keV.

5 Input

Input files should be placed in the directory `$EGS_HOME/backscatter_clrp`. An input file uses a "delimiter" to search for a particular group of entries. If the required input is not found between the `Start` and the `Stop` of the delimiter, an error message is generated and the code may exit if the simulation is not able to proceed without the missing input. Individual entries within a delimiter group must be preceded by a particular string with an equal sign next to it (with no space). The code uses these strings to search for the values of the entries. The order of entries in a particular delimiter group is not important. Table 2 shows two sample input files included in the package of the user-code `backscatter_clrp`. The following is a description of these two sample input files.

Table 2

• **Incident charged particle beam:** The inputs must be placed between the `Start` and the `Stop` of the delimiter `charged particle beam input`. The inputs are: the charge of the particles in the beam (-1 for electrons and +1 for positrons), the kinetic energy of the incident particles (in keV), the angle of incidence from the normal (in degrees) and the total number of incident charged particles, i.e. the number of histories. The first sample input file has a monoenergetic pencil beam of 5 million electrons with a kinetic energy of 60.0 keV incident on a target at an angle of 55.0° from normal. The second sample input file has a monoenergetic pencil beam of 10 million positrons with a kinetic energy of 50.0 keV normally incident on a target.

Table 2: Two sample input files for the user-code backscatter_clrp.

Sample Input File 1
sample_input_01.egsinp

```
========================================
:Start charged particle beam input:

Incident charge=             -1
Kinetic energy (keV)=      60.0
Incidence angle (degrees)= 55.0
No. histories=          5000000

:Stop charged particle beam input:
========================================

========================================
:Start target input:

Materials=                Ag
Layer thickness (cm)=   20.0
Layer material=            1

:Stop target input:
========================================

========================================
:Start backscatter coefficient input:

Backscatter coefficient= On

:Stop backscatter coefficient input:
========================================

========================================
:Start energy spectra input:

Method of input= individual
Phi (degrees)=      0.0, 20.0,  90.0
Theta (degrees)=  -67.5,  0.0,  20.0
Solid angle (msr)= 10.0, 75.0, 150.0

No. energy bins=                  60
Overall energy spectrum=          On

:Stop energy spectra input:
========================================

========================================
:Start angular distributions input:

Phi (degrees)=       0.0,  45.0,  90.0
Solid angle (msr)= 100.0, 100.0, 100.0

No. angular bins=                   90

:Stop angular distributions input:
========================================

========================================
:Start MC transport parameter:

Global ECUT=                   0.512
Global PCUT=                   0.001
Bound Compton scattering=         On
Rayleigh scattering=              On
Atomic relaxations=               On
Photoelectron angular sampling=   On
Brems angular sampling=       Simple
Spin effects=                     On
Electron impact ionization=       On
Photon cross sections=          xcom

:Stop MC transport parameter:
========================================
```

Sample Input File 2
sample_input_02.egsinp

```
========================================
:Start charged particle beam input:

Incident charge=              +1
Kinetic energy (keV)=       50.0
Incidence angle (degrees)=   0.0
No. histories=          10000000

:Stop charged particle beam input:
========================================

========================================
:Start target input:

Materials=                       Al, Cu
Layer thickness (cm)= 1E-3, 1E-3, 20.0
Layer material=          1,    2,    1

:Stop target input:
========================================

========================================
:Start backscatter coefficient input:

Backscatter coefficient= Off

:Stop backscatter coefficient input:
========================================

========================================
:Start energy spectra input:

Method of input= groups
Phi (degrees)=      10.0, 43.0, 75.0
No. detectors=         7,    5,    3
Solid angle (msr)= 100.0, 60.0, 90.5

No. energy bins=                  25
Overall energy spectrum=         Off

:Stop energy spectra input:
========================================

========================================
:Start angular distributions input:

Phi (degrees)=       0.0,  30.0
Solid angle (msr)= 150.0, 150.0

No. angular bins=           180

:Stop angular distributions input:
========================================

========================================
:Start MC transport parameter:

Global ECUT=                   0.513
Global PCUT=                   0.002
Bound Compton scattering=         On
Rayleigh scattering=              On
Atomic relaxations=               On
Photoelectron angular sampling=   On
Brems angular sampling=       Simple
Spin effects=                    Off
Electron impact ionization=      Off
Photon cross sections=          xcom

:Stop MC transport parameter:
========================================
```

• **Target:** The front surface of the target lies in x-y plane with z = 0. The depth of the target increases in the +z direction. The inputs for the target must be placed between the Start and the Stop of the delimiter target input. The inputs are: the materials making all the layers of the target, the thickness of each layer (in cm) and the material number for each layer. The materials can be elements, mixtures or compounds and their data must be included in the .pegs4dat file that will be used in the simulation. Material names are case-sensitive, therefore they must exactly match their entry in the .pegs4dat file. The target can be made of a single thick layer (bulk target), multiple thin layers on a substrate (composite targets) or self-supporting thin layers (thin film targets). The first sample input file has an semi-infinite silver target (semi-infinite because 20 cm is much larger than the range of 60.0 keV electrons in silver). The second sample input file has a composite target made of a 10 μm aluminum film followed by a 10 μm copper film and both are deposited on an infinitely-thick aluminum substrate.

• **Backscatter coefficient:** The inputs must be placed between the Start and the Stop of the delimiter backscatter coefficient input. The backscatter coefficient is sought in the first sample input file and is not in the second.

• **Energy spectra of backscattered charged particles:** The inputs must be placed between the Start and the Stop of the delimiter energy spectra input. The location of a counting detector to measure an energy spectrum is fully characterized by the plane angle, ϕ, and the backscatter angle, θ. The solid angle subtended by the detector, with respect to the center of the target surface, is also needed for the simulation. There are two methods for entering detector data: individual and groups. For individual, individual detector locations and solid angles are entered. For groups, a backscatter plane is specified using ϕ, and a certain number of detectors is uniformly distributed on that plane. All detectors in a given plane must have the same solid angle. In the first sample input file, the energy spectra at three individual locations are sought, and the location and solid angle of the detectors used are given. In the second sample input file, the variation of the energy spectra versus the backscatter angle, θ, is sought for three planes. For example, the second plane is at $\phi = 43.0^\circ$ and five detectors, each of them subtends a solid angle of 60 msr, are placed uniformly in that plane at $\theta = -72^\circ$, -36°, 0°, 36° and 72°, respectively. The overall energy spectrum, i.e. using a hemispherical detector, is sought in the first sample input file and is not sought in the second. The user can also get the overall energy spectrum without any other individual or group detectors. The energy spectra are in 1.0 keV bins in the first sample input file (60.0 keV/60 bins) and in 2.0 keV bins in the second (50.0 keV/25 bins).

• **Angular distributions of backscattered charged particles:** The inputs must be placed between the Start and the Stop of the delimiter angular distributions input. The inputs are: the backscatter planes, the solid angle of the detectors used in each plane and the number of angular bins, i.e. the number of detectors in the plane. In the first and second sample input files, the angular distributions are sought for three planes and for two planes, respectively. Angular distributions are in 2.0° bins (180°/90 bins or detectors) in the first sample input file and in 1.0° bins (180°/180 bins or detectors) in the second.

If the user is interested in only one or two types of output (e.g., only backscatter coefficient or only backscatter coefficient and angular distributions) then the block(s) that is(are) not of interest must be deleted from the input file (including the delimiters). The maximum numbers allowed for target materials, planes of backscatter, detectors, energy bins and angular bins are 10, 10, 1800, 300 and 180, respectively. These values can be increased or decreased by changing the parameters `$MXMED`, `$MXPLN`, `$MXDET`, `$MXBINE` and `$MXBINA` at the beginning of the source file `backscatter_clrp.mortran` then re-compiling the code as explained in section 3.

• **Monte Carlo transport parameters:** The inputs must be placed between the `Start` and the `Stop` of the delimiter `MC transport parameter`. The user needs to specify the cut-off energies (in MeV) for photons and charged particles below which their transport is terminated and their energy is deposited locally. The user also has the option to specify the low-energy physics to be included in the simulation. The transport parameters shown in the two sample input files are the most relevant ones to low-energy applications - see the EGSnrc manual[4] for the other parameters that the user has the option to control. If an entry for one of the transport parameters is missing, EGSnrc uses a default value - see the EGSnrc manual[4] for these defaults. In the first sample input file, electrons are tracked down to a kinetic energy of 1 keV, i.e. to a total energy of 0.001 + 0.511 = 0.512 MeV and photons to an energy of 1 keV. All low-energy physics available in EGSnrc are turned `On` and the `XCOM` cross section data are used for photons. In the second sample input file, positrons, electrons and photons are tracked down to a kinetic energy of 2 keV. Electron impact ionization and electron spin effects are turned `Off`. This could be used to study the effect of these two physics processes on the backscatter output.

6 Output

After a successful simulation, a `.errors` file and a `.egslst` file can be found in `$EGS_HOME/backscatter_clrp`. The `.errors` file has a list of errors encountered while reading the input file. It can be used to identify problems with the input. The `.egslst` file contains an echo of the inputs, a visual schematic of the layers of the target, the full list of the transport parameters used in the simulation and the output requested by the user which could be any combination of the charged particle backscatter coefficient, the energy spectra at the detector locations specified by the user, and the angular distributions in the backscatter planes specified by the user. For the energy spectra and angular distributions, the independent variable represents the value at the *center* of the bin. The statistical uncertainty is reported for all output quantities.

7 Limitations

• Splitting a simulation into multiple parallel runs is not available for the user-code backscatter_clrp.

• Detector response at the locations specified by the user is not simulated. An ideal counting detector is assumed.

• Results for incident beams of charged particles with kinetic energy $\leq$ 10 keV are affected by the limitations of the underlying theoretical models used in EGSnrc.[1,2]

• The lowest kinetic energy cut-off is 1 keV. Therefore, a cut-off of 50 eV, corresponding to the retarding grid bias, is not possible. We discussed the systematic uncertainties introduced by the 1 keV kinetic energy cut-off elsewhere.[1,2]

8 References

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