PolEM
Polarized Electron Mott Scattering Model User's Manual

Michał Drągowski
mdragowski@fuw.edu.pl

December 31, 2020

1 Package Contents

The interaction model distribution package contains the following directory structure:

```
PolEM/
|-> include/
|-> src/
|-> data/
|-> generator/
|-> manual/
```

Files from the `include` and `src` directories should be placed in the header and source directories of your Geant4 simulation project. They will be compiled together with your simulation code, so there is no need to modify the core Geant4 installation.

In order to use the pre–generated data files, the complete `data` directory should be copied to the directory with your simulation executable. It contains data generated with the error correction switched on for the following elements: gold (for energies from 1 keV to 10 MeV, with the muffin–tin model), lead (from 1 keV to 14 MeV, with the muffin–tin model), and for hydrogen – component of vacuum in Geant4 (from 1 keV to 14 MeV). This way there is no need to compile and run the cross section generator.

In order to generate custom cross section files, the code from the `generator` directory should be compiled with a FORTRAN compiler (e.g., gfortran), see below for details.

The `manual` directory contains this file.

2 Using the Model with Geant4

The Mott scattering interaction model can be included in the simulation by constructing a custom physics list, inheriting from a base Geant4 class `G4VUserPhysicsList`. After including the model files with

```
#include "MottScatteringModel.hh"
```

an instance of the Mott scattering model can be created in the `ConstructProcess()` method with

```
MottScatteringModel* mott = new MottScatteringModel();
```

Then, it can be set as a model of Coulomb scattering with

```
G4CoulombScattering* coulomb = new G4CoulombScattering();
coulomb->SetEmModel(mott, 1);
```

The standard Geant4 methods for setting energy cuts should be used to make sure that the energy range, in which the model is applied, matches the range of the cross section files. This can be done with

```
coulomb->SetMinKinEnergy(1.*keV);
coulomb->SetMaxKinEnergy(100.*keV);
```

Note also that, depending on the Geant4 version, it might be necessary to explicitly set the scattering angle range with

```
G4EmParameters* param = G4EmParameters::Instance();
param->SetMscThetaLimit(0.);
```

see [section VI. D. in Sung Hun Kim et al., *IEEE Trans. Nucl. Sci.* 62, 451 (2015)] for more details.

3 Additional Features of the Model

In the `MottCrossSection.cpp` file there are two flags which can be uncommented to switch on additional features:

1. The `PolEM_CORRECT` flag switches on the data correction algorithm, which interpolates the data tables imported from ELSEPA if inconsistencies are found. The same algorithm is included in the cross section generator, so it makes sense to uncomment the flag only if the input data were generated without corrections.

2. The `PolEM_CSDA` flag switches on a continuous energy loss proportional to the path length, according to the average energy loss files `csdaZ.dat`, where `Z` is the atomic number. The files should be placed in the `data` directory and contain two columns: electron energy and average energy loss in keV/nm/(g/cm3). The data can be downloaded from the ESTAR database [M.J. Berger, J.S. Coursey, M.A. Zucker, J. Chang, NIST Stopping–Power and Range Tables for Electrons, Protons, and Helium Ions, Available from: http://www.nist.gov/pml/data/star/index.cfm]. This feature is only for testing purposes; under normal conditions the energy loss should be taken into account by including the ionization and bremsstrahlung processes in the physics list.

4 Using the Cross Section Generator

Some of the cross section generator settings can be controlled with the `control.inp` file, without re–compiling the code. The following parameters are available:

- maximum energy,

- minimum energy,

- target atomic number,

- muffin–tin model (on/off flag),

- error correction (on/off flag).

After running the generator, the data files are stored in the `generator/data` directory, which must then be copied to the directory with the Geant4 simulation executable.

The error correction function simply interpolates the data from the neighboring points if an inconsistency is found in the ELSEPA output. If the interpolation is unsuccessful in a few iterations, then extrapolation from previous points is performed.

The control plots corresponding to Figure 2 in [M. Drągowski et al., Nucl. Instr. Meth. B 488, 37 (2021)] are shown on the next page for uncorrected and corrected data. The errors in uncorrected data are clearly visible. After correction there are no inconsistencies noticeable in the plots.
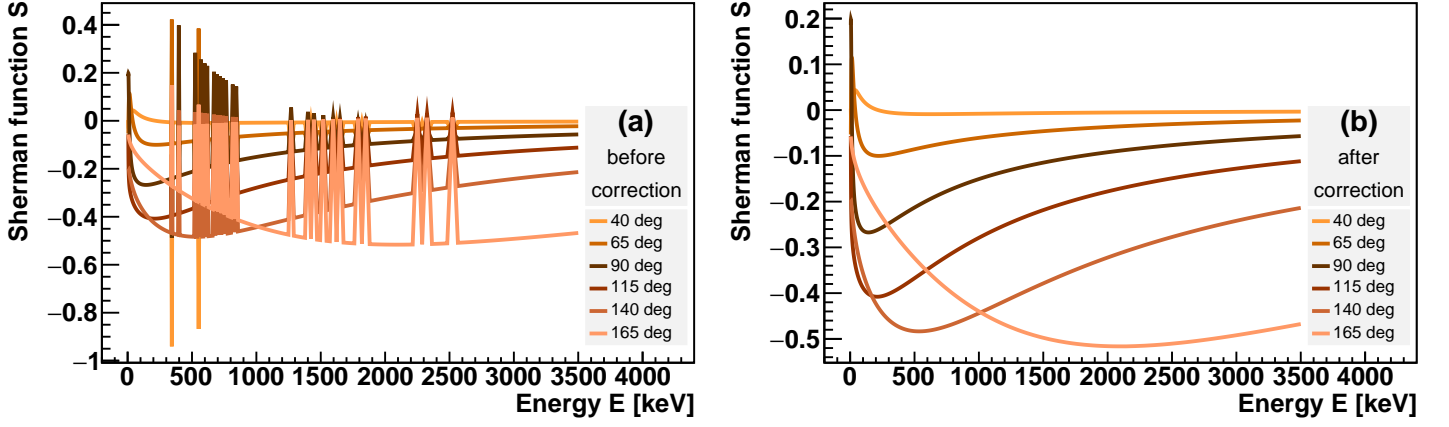
Figure 1: Dependence of the theoretical Sherman function S on electron energy E for electron scattering off gold atoms generated with ELSEPA. Left (a): raw data. Right (b): after corrections.
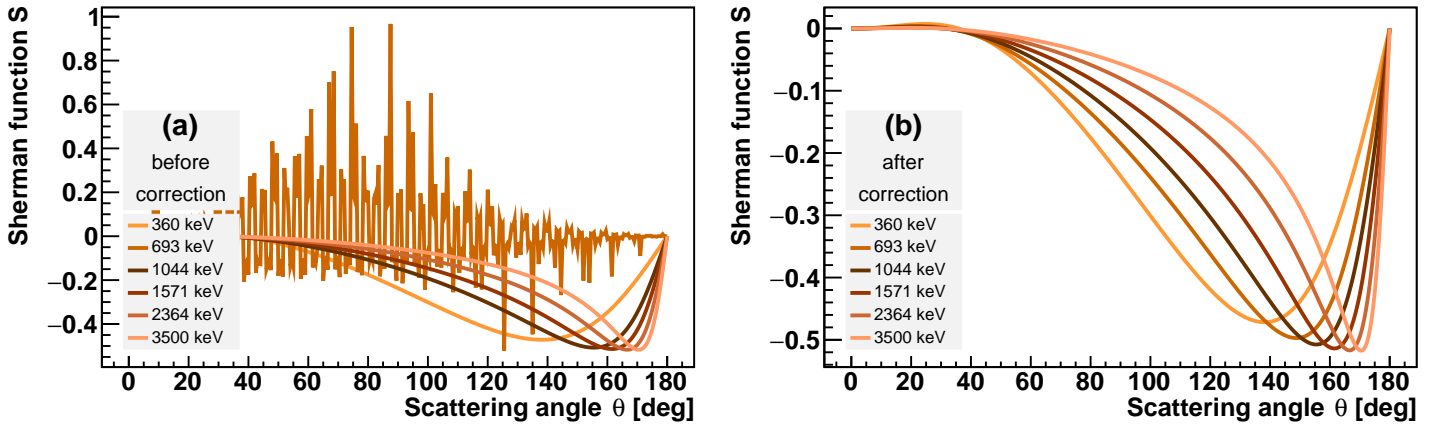

Figure 2: Dependence of the theoretical Sherman function S on the scattering angle θ for electron scattering off gold atoms generated with ELSEPA. Left (a): raw data. Right (b): after corrections.