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Title: ELECTRON TRANSMISSION AND BACKSCATTER VERIFICATON CALCULATIONS USING MCNP5

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ELECTRON TRANSMISSION AND BACKSCATTER VERIFICATON CALCULATIONS USING MCNP5

By

Phuongloan Libby, Grady Hughes, and John T. Goorley

Abstract

This paper shows a comparison of simulated electron transmission and backscatter experiments using MCNP5, to calculations with MCNP4B by D. P. Gierga and K. J. Adams[3], and data by Ebert *et al.*[2] experiments. The experiments are for 4.0-12.0 MeV monoenergetic electrons incident on a variety of thin disk targets. The MCNP5 simulations used 6.0, 8.0, and 10.2 MeV monoenergetic electrons incident on three materials: carbon (*C*), silver (*Ag*) and uranium (*U*), at a thickness of 0.46279 cm. Different carbon densities were used for MCNP5 simulations due to the lack of reported density information from the references. The densities are 1.7g/cc (graphite), 2.0g/cc (amorphous carbon), and 2.267g/cc (elemental carbon). There is no agreement found of transmission coefficient through *Ag* and *U* targets. For elemental *C*, at all three electron energies a closer agreement found between the MCNP5 simulations and Ref. 2 values, to within one standard deviation, $\pm 1\sigma$, of the experimental and calculated errors. The backscatter coefficient results are varied for different targets. For *Ag* and *U*, the agreement between Ref. 2 and MCNP5 values is within $\pm 2\sigma$ and within $\pm 1\sigma$ of the two MCNP versions. For carbons, there is no agreement found between the two MCNP versions. The agreement between MCNP5 and Ref. 2 values is within $\pm 1\sigma$ for elemental *C* and within $\pm 2\sigma$ for graphite and amorphous carbon.

Introduction

In 1999, D. P. Gierga and K. J. Adams authored *Electron/Photon Verification Calculations Using MCNP4B* which used Ebert *et al.* [2] as a benchmark. Since then there is no electron benchmark calculations performed to reassuring the results from MCNP4B. Therefore, an extension of their study, [2,3] was performed using MCNP5 to focus on electron transmission and backscatter calculations. A set of electron transmission and backscatter experiments was simulated using the same input deck to MCNP4B with minor modifications. The MCNP5 simulations included 6.0, 8.0 and 10.2 MeV monoenergetic electrons incident on three thin disk materials: carbon (*C*), silver (*Ag*) and uranium (*U*), at a thickness of 0.446 cm. Multiple carbon densities (graphite (1.7g/cc), amorphous carbon (2.0g/cc), and elemental carbon (2.267g/cc)) were used for the simulations due to the lack of reported density information by the references. The results presented in this paper are compared with Ebert's data and Gierga and Adams' simulated, MCNP4B, results.

For the transmission coefficients through Ag and U targets, there is no agreement found. For elemental *C*, at all three electron energies a closer agreement found between the MCNP5 simulations and Ref. 2 values, to within one standard deviation, $\pm 1\sigma$, of the experimental and calculated errors.

For the backscatter coefficient, the agreement between experiment and simulations are varied. The electron backscatter results from *Ag* and *U* are within $\pm 1\sigma$ between the two Monte Carlo code versions and are within $\pm 2\sigma$ comparing with Ebert's data. For carbons, there is no agreement found between the two MCNP versions. The agreement between MCNP5 and Ref. 2 values is within $\pm 1\sigma$ for elemental *C* and within $\pm 2\sigma$ for graphite and amorphous carbon.

The rest of this report discusses the Ebert *et al.* experimental methods, the MCNP5 simulation descriptions and the simulated results and analysis.

Ebert *Et Al.*, Experimental Methods

Ebert *et al.*, gives a tremendous amount of transmission and backscatter data for 4.0, 6.0, 8.0, 10.2, and 12.0 MeV monoenergetic electrons incident on a variety of solid

targets. In this study, a few of the transmission and backscatter experiments, 6.0, 8.0, and 10.2 MeV electrons, have been simulated using MCNP5.

A beam of electrons of current I_o (C/s) incident on a planar target is subjected to measure for backscattered, absorbed, and transmitted coefficients. During some time τ (s), a charge $Q_o = I_o\tau$, in Coulombs, is incident on the target. The transmission coefficient T is given by

$$T = \frac{Q_T}{Q_o} = \frac{Q_T}{Q_B + Q_A + Q_T}, \tag{1}$$

where Q_T is the charge transmitted through the target, Q_A is the charge absorbed in the target, and Q_B is the charge backscattered from the target. The backscatter coefficient B is given by

$$B = \frac{Q_B}{Q_o} = \frac{Q_B}{Q_B + Q_A + Q_T}. \tag{2}$$

The target chamber contained x-ray shielding, two large Faraday cups, and a carbon beam stop in addition to the collimator assembly. The Faraday cups were used to collect the transmitted and backscattered electrons. Bias rings, set to 500 V, were mounted in the Faraday cups to minimize the very low energy secondary electron current. The target dimensions were chosen such that the target radius was greater than the sum of the beam radius and the maximum electron range, (Ref. 3). The experimental geometry is shown in Figure. 1.

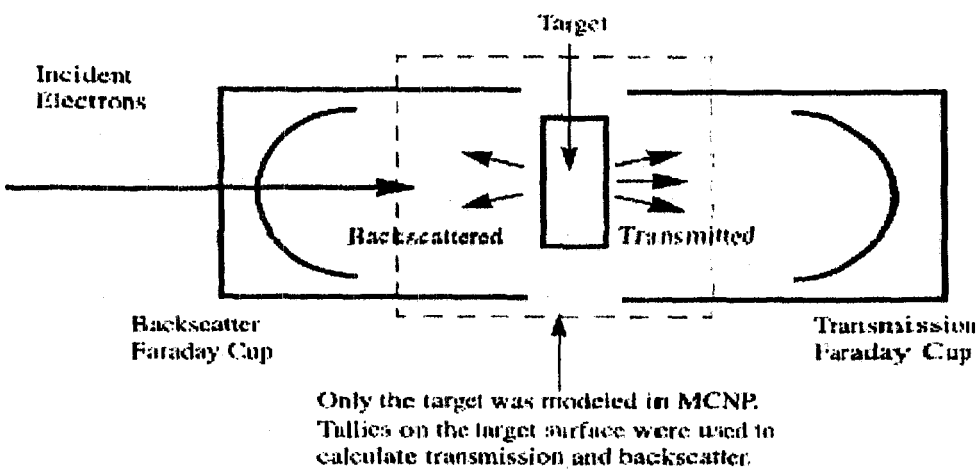

Figure 1. Geometry of Ebert transmission and backscatter experiments.

MCNP5 Simulation Descriptions

This section of the report describes the problem geometry, the source definition, the problem tallies, and the executable command used on Lambda, one of Los Alamos National Laboratory's supercomputers. This information provides insight into the fundamental properties of Monte Carlo electron transport.

The experimental geometry was greatly simplified for the MCNP5 simulations, Figure 2. In this configuration, only the target was explicitly modeled. According to Gierga and Adams, this technique is much simpler than modeling the Faraday cup geometry, and ensures that there are no tally losses from solid angle effects. The transmission and backscatter coefficients were calculated using current tallies at the target faces.

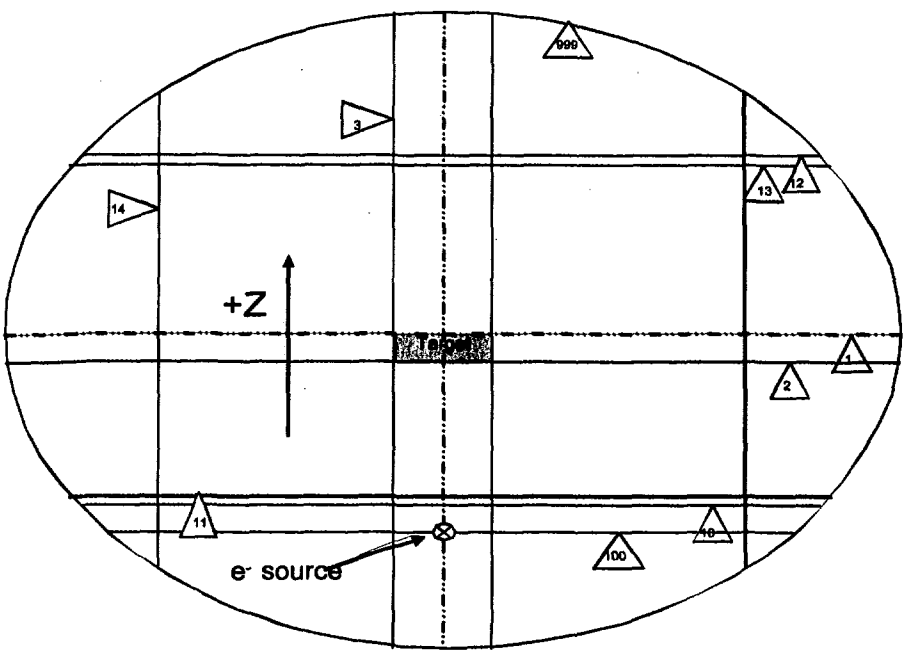

Figure 2. Geometry of MCNP5.

In Figure 2, all triangle icons label the surfaces number accordingly to the MCNP5 input deck, Appendix A, which is the same input deck from MCNP4B, Appendix B, with minor modifications. The only change added was a RAND card with different stride number, (stride = 152,917,777), due to a warning from MCNP5 that the default random number was exceeded.

All surfaces are at fixed location for this problem (surface 2 was adjustable to change the target thickness for Geirga and Adams, 1999). Inside surface 999, a 100 cm radius sphere, is vacuums, except for the target. The target is 0.46279 cm thick and is bounded by surface 1, 2 and 3. The source is a 6.0, 8.0, and 10.2 MeV electrons pencil beam, 0.3cm in radius, and is located on the z-axis 11.0 cm away from the top target surface (surface 1).

The current tallies were divided into two cosθ bins, where θ is defined relative to the positive surface normal. The transmission coefficients were calculated by using a θ range of 0° to 90° and measured, using MCNP5, by current tallies on surface 1 and 3, (*f31:e 1* and *f41:e 3*). The backscatter coefficient was calculated using a θ range of 90° to 180° and measured, using MCNP5, by current tally on surface 2, (*f1:e 2*). The simulations were done in coupled electron/photon mode, used the default low energy cutoffs of 1 keV, and the physics with full Bremsstrahlung treatment.

All simulations were executed on Lambda using the command: *bsub –n* #of processors *–o out*.name *–q large2q mpijob mpirun /users/libby/bin/mcnp5.run name*=filename *balance eol*. Lambda is an unclassified general compute resource. It consists of 328 Intel Pentium 3 processors across 164 compute servers running Redhat Linux (*2.4.18 #1 SMP Mon Nov 4 11:09:23 MST 2002 i686*). *LeheyFortran95Pro* compiler version *6.2*, *mpich 1.2.3.absoft_7.5*, was loaded after the *bsub* command was executed. The thread name and version used for each run was MCNP5_LANL, 1.14. There was no module loaded for these simulations.

Neither Gierga and Adams nor Ebert *et al.* reported the material densities used for their inputs. This work used the following densities for *Ag* and *U*: 10.48 and 19.0 g/cc, respectively. For *C*, there are multiple densities available: 1.7 g/cc (graphite), 2.0 g/cc (amorphous carbon), and 2.267g/cc (elemental carbon). The MCNP5 simulations used all three densities.

Results & Analysis

This section presents the results of MCNP5 simulations besides analyzing the output parameters.

For all runs, 40-60 processors were used. The computer time ranged from 16 to 375 minutes. The longer runs belonged to the higher Z material, *U*, and the higher energy source due to Bremsstrahlung cascading effect. All simulations used 1.5E6 particles, (nps = 1.5e6), except some runs needed to run longer to pass the slope test, which required 2.0E6 particles. These are including 6.0 and 10.2 MeV incident electrons on carbons. At 6.0 MeV incident electrons on graphite, there are two statistical checks did not pass from tally 41, the mean behavior and the figure of merit, FOM, behavior. At 6.0 and 10.2 MeV incident electrons on amorphous carbon, the mean behavior did not pass from tallies 31 and 41, respectively. Table 1 summarizes the input parameters of different target:

Table 1. Target's parameters for MCNP5 input

Parameters	C	Ag	U
R (cm)	1.000	1.000	1.000
H (cm)	0.463	0.463	0.463
A(cm^2)	9.191	9.191	9.191
V(cm^3)	1.454	1.454	1.454
ρ (g/cm^3)	2.267	10.480	19.000
m (g)	3.296	15.237	27.624
t (g/cm^2)	0.359	1.658	3.006

Transmission coefficients were graphically presented as a function of targets thickness in Ref. 2&3. At the calculated thickness specified in Table1, the transmission coefficient values were reading off the graphs for reference values. The MCNP5 simulated results is compared with these reference values in Table 2:

Table 2. Transmission Coefficient Comparison

Material	e's E (MeV)	MCNP5	% Error	Ebert	% Error	% different	MCNP4B	% different
Elem. C	10.2	1.07E+00	0.02	1.08	1.5	0.01	1.03	0.03
Ag		4.96E-02	0.37	0.87	1.5	0.94	0.95	-18.15
U		8.77E-03	0.82	0.22	1.5	0.96	0.205	-22.38
Elem. C	8	1.06E+00	0.02	1.07	1.5	0.01		
Ag		5.86E-03	1.37	0.7	1.5	0.99		
U		4.77E-03	1.55	0.05	1.5	0.90		
Elem. C	6	1.05E+00	0.02	1.05	1.5	0.00		
Ag		2.52E-03	1.69	0.32	1.5	0.99		
U		2.45E-03	1.74	0.01	1.5	0.76		

Table 2 shows no agreement between MCNP5 to either Ebert or MCNP4B results on *Ag* and *U*. However, Figure 3 shows a close agreement for elemental carbon compared with Ebert's data, within -1σ.

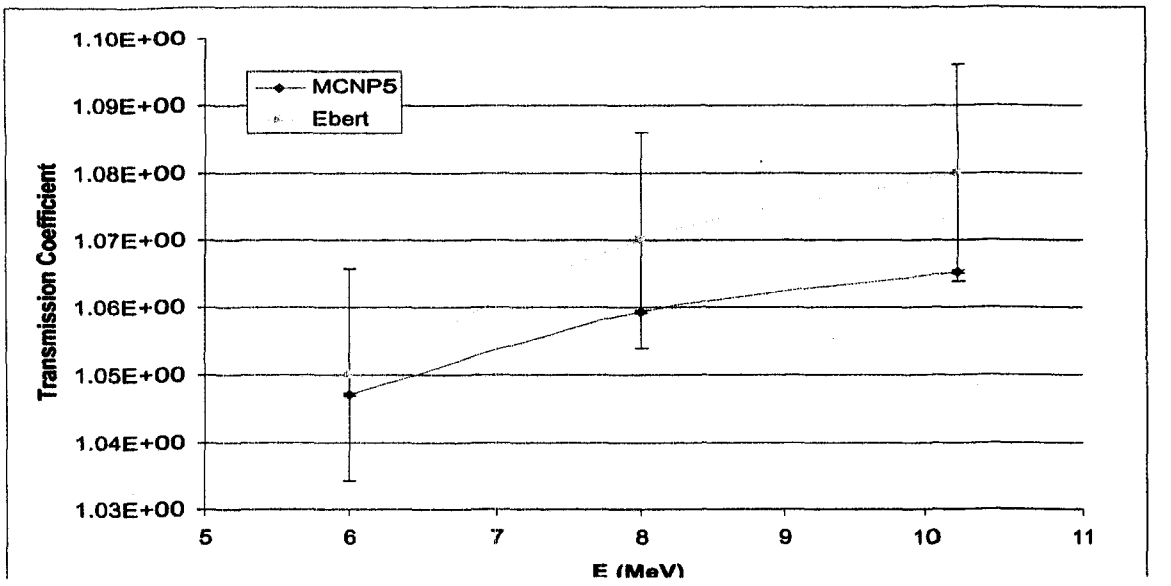

Figure 3. Electron transmission coefficient through elemental *C* target.

Graphically, we can see in Figure 4 that the transmission coefficient increases as the electron energy increases and the target density decreases. This agrees well with the fact that it is harder to transmit lower electrons energy through a denser material.

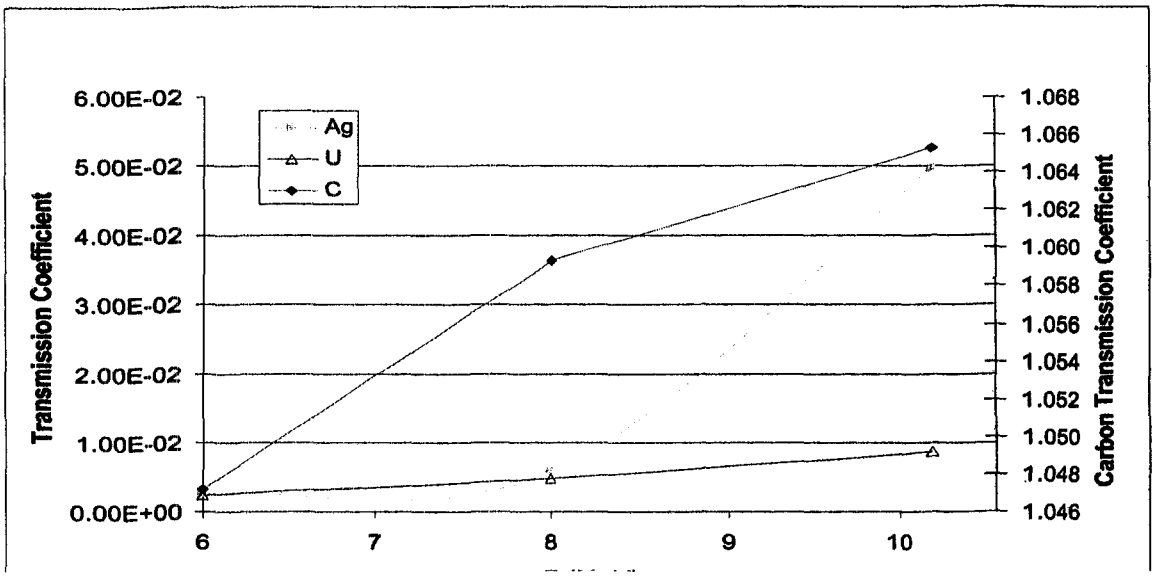

Figure 4. Transmission Coefficient on Elemental Carbon, Silver, and Uranium.

Tables 3, 4 & 5 show the results of the backscatter benchmark calculations for *Ag*, *U* and *C*, respectively. The values in parentheses for the Monte Carlo simulations are the percent errors. Data from Dressel[1] and Tabata[4] are also included to show the wide range of experimental values that are in the literature.

Table 3. Electron Backscatter Comparison for Ag

Material	e's E (MeV)	Ebert	Dressel	Tabata	MCNP4B	MCNP5
Ag	6	1.39E-01(8.0)	2.40E-01	1.29E-02	1.50E-01(2.0)	1.54E-01(0.20)
Ag	8	9.50E-02(8.0)	2.00E-01	9.70E-02	1.15E-01(2.0)	1.16E-01(0.29)
Ag	10.2	7.40E-02(8.0)	1.80E-01	7.35E-02	8.47E-02(3.0)	8.78E-02(0.28)

Table 4. Electron Backscatter Comparison for U

Material	e's E (MeV)	Ebert	Dressel	Tabata	MCNP4B	MCNP5
U	6	2.45E-01(8.0)	4.50E-01	2.28E-01	2.78E-01(1.01)	2.78E-01(0.14)
U	8	1.95E-01(8.0)	3.80E-01	1.72E-01	2.18E-01(2.0)	2.22E-01(0.20)
U	10.2	1.47E-01(8.0)	3.30E-01	1.36E-01	1.78E-01(2.0)	1.80E-01(0.16)

Table 5. Electron Backscatter Comparison for C

Published Data				MCNP5		
Material	e's E (MeV)	Ebert	MCNP4B	Elemental C	Amorphous C	graphite
C	6	6.00E-03(8.0)	6.86E-03(3)	6.00E-03(1.08)	5.51E-03(0.97)*	5.12E-03(1.01)*
C	8	5.00E-03(8.0)	6.12E-03(4)	5.03E-03(1.18)	4.76E-03(1.21)	4.59E-03(1.23)
C	10.2	4.00E-03(8.0)	5.85E-03(4)	4.64E-03(1.22)	4.64E-03(1.06)*	4.56E-03(1.23)

Backscatter coefficient comparisons of MCNP5 results, from *Ag* and *U* targets, to the references are graphically presented in Figures 5 & 6. These show the agreement between the two MCNP versions within ±1σ and within ±2σ between Ebert data and MCnP5 results.

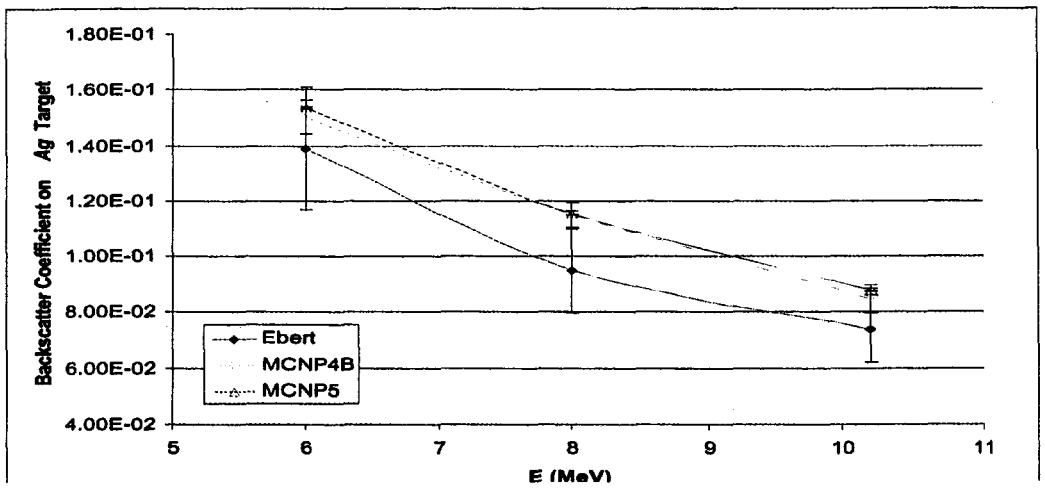

Figure 5. Electron backscatter coefficient through elemental *Ag* target.

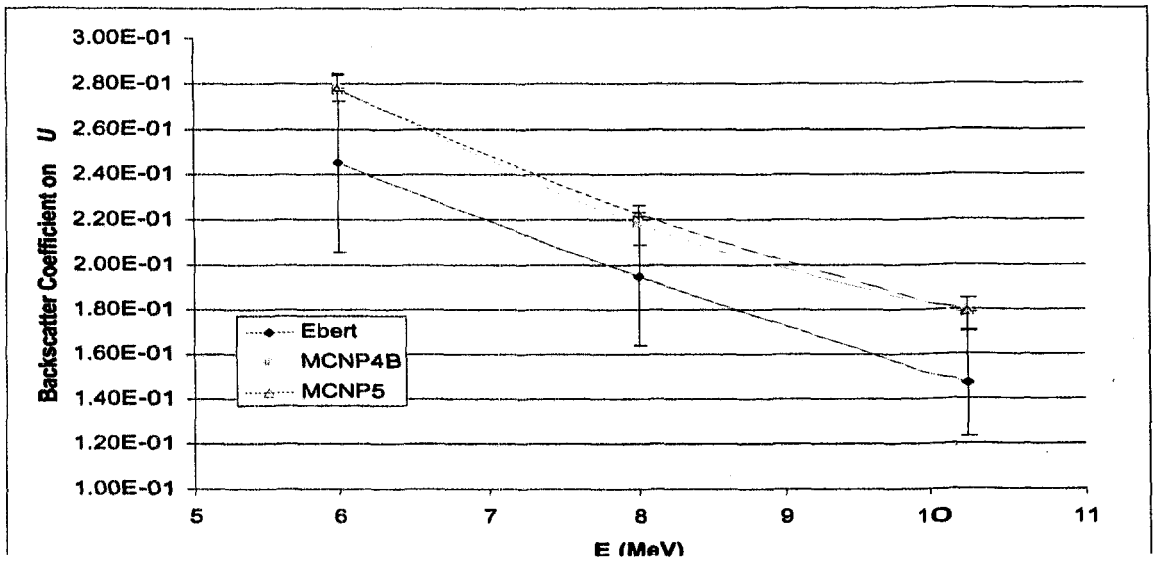

Figure 6. Electron backscatter coefficient through elemental U target.

Carbon target was simulated with three different densities: 1.7g/cc (graphite), 2.0 g/cc (amorphous carbon), and 2.267 g/cc (elemental *C*). The results compared with Ebert and MCNP4B presented graphically in Figure 7.

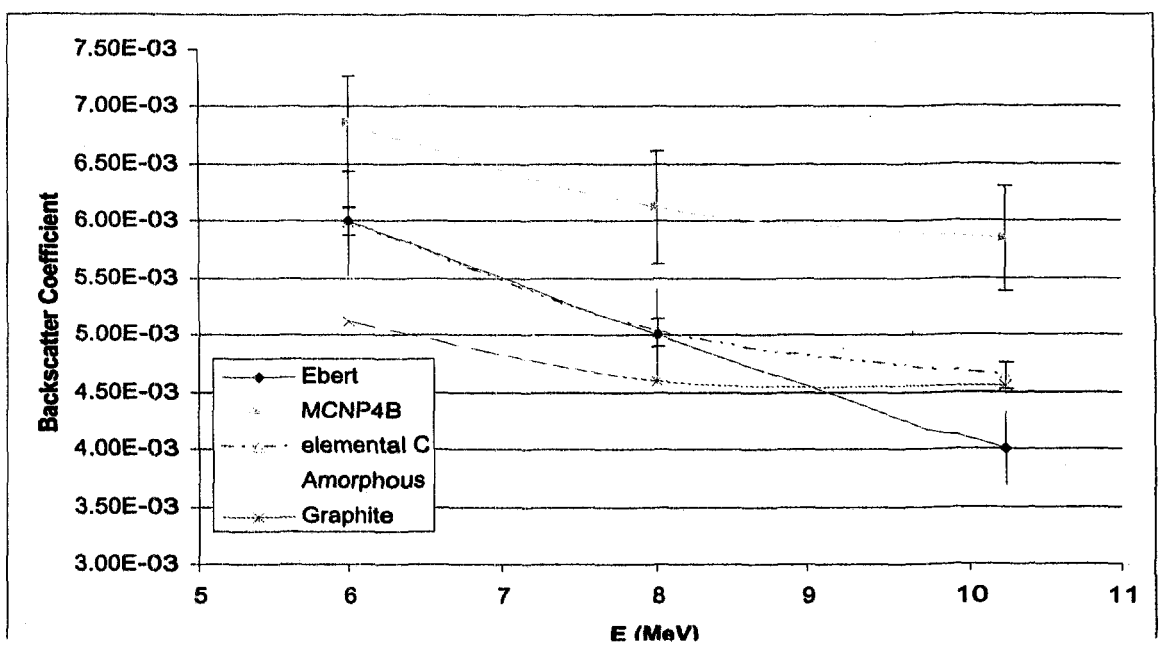

Figure 7. Comparison of backscatter coefficient through carbons target.

The above figure shows no agreement between the two Monte Carlo code versions for the backscatter coefficient through carbons target. However, closer agreement found comparing with Ebert data. Elemental *C* has the closet agreement to within $\pm 1\sigma$ and within $\pm 2\sigma$ for graphite and amorphous carbon.

For *Ag* and *U*, Table 6 shows the default MCNP5 simulations agree with the Ebert *et al.* experiment to within 10-18%, which is better than Gierga and Adams, 8-20%, and the MCNP4B simulations to within 0-4%. For elemental carbon, the default MCNP5 agrees well with Ebert *et al.* experiment to within 0-14%.

Table 6. Percentage Difference between MCNP Simulations & Ebert *et al.* Experiment

Material	e's Energy (MeV)	MCNP4B & Ebert	MCNP5 & Ebert	MCNP5 & MCNP4B
Elemental carbon	6	0.12	0.00	0.13
Ag		0.08	0.10	0.02
U		0.12	0.12	0.00
Elemental carbon	8	0.18	0.01	0.18
Ag		0.17	0.18	0.01
U		0.11	0.12	0.02
Elemental carbon	10.2	0.32	0.14	0.21
Ag		0.13	0.16	0.04
U		0.17	0.18	0.01

Figure 8 shows a graphical backscatter coefficient comparison between *C, Ag,* and *U* target:

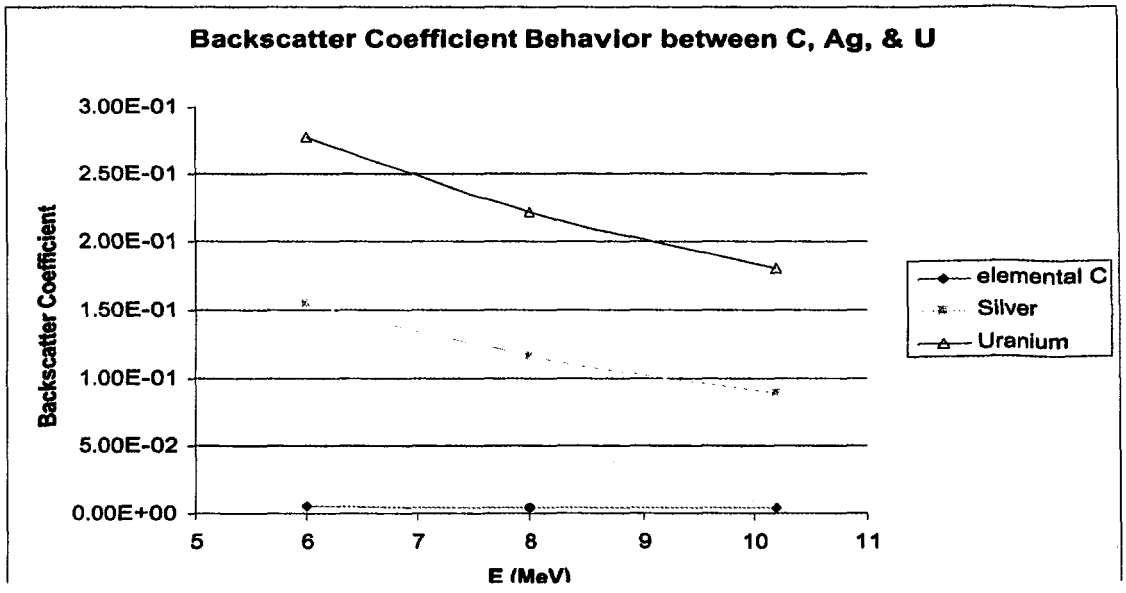

Figure 8. Backscatter Coefficient on Elemental Carbon, Silver, and Uranium

It is observed that, as the electron energy increases, the backscatter coefficient decreases, and it is increases as the target density increases. This is opposite to the transmission coefficient behavior, which is expected. A denser material has more possibility to create more backscatter particles as it is collided with the target nucleus. With the same principal, this behavior can be observed more clearly in Figure 9, which is comparing the backscatter coefficient of carbon at different density.

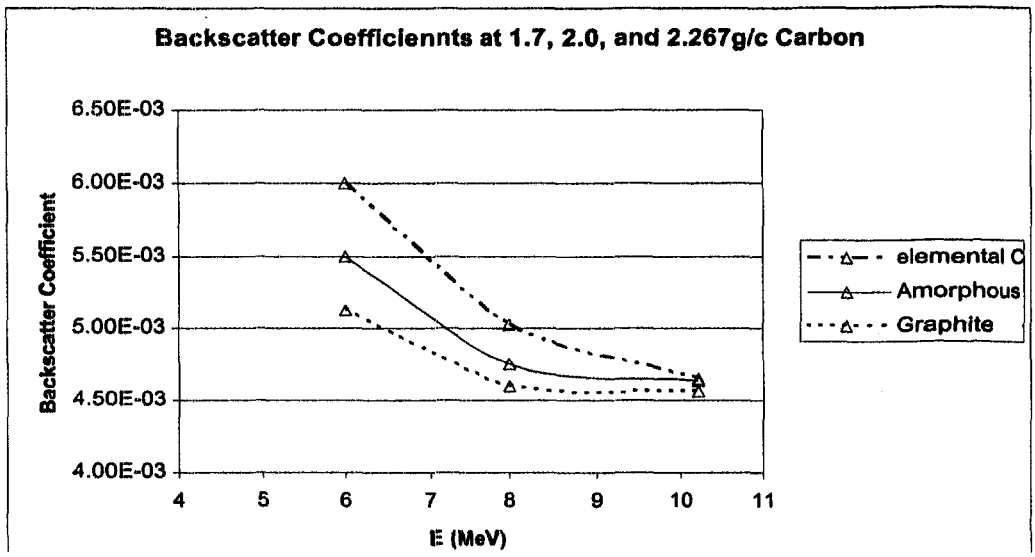

Figure 9. Carbons' Backscatter Coefficients

The above figure shows that, there is more back scatter at higher density material. However, at higher electron energy, the backscatter coefficient is lower. This behavior confirms that, at higher energy, electrons have more possibility to transmit through material than backscatter.

Conclusions

MCNP5 was verified against a series of electron/photon transmission and backscatter experiments. These verification calculations agreed with experiment within 10-18% and within 0-4% comparing with MCNP4B simulation for *Ag* and *U*. For *C*, poor agreement was found at lower densities, 1.7g/cc and 2.0g/cc, but well agreement was found for 2.27g/cc to compare with Ebert *et al.*'s experiment. The overall agreement suggested that electron transmission and backscatter calculations in MCNP still required improvement. More computer time should be invested in the calculations presented here to assess the statistical convergence of the differential energy spectra. Finally, more benchmark studies at lower and higher electron energies should be performed and compared to a wider range of experiments.

References

1. Dressel, R. W., "Retrofugal Electron Flux from Massive Targets Irradiated with a Monoenergetic Primary Beam," Phys. Rev. 144, pp. 332-343, 1966.
2. Ebert, P.J., Lauzon, A. F., and Lent, E. M., "Transmission and Backscattering of 4.0-12.0 MeV Electrons, " Phys. Rev. 183, 1969, pp. 422-430.
3. Gierga, D. P. and Adams, K. J., "Electron/Photon Verification Calculations Using MCNP4B," Los Alamos National Laboratory, Los Alamos, New Mexico 87545, LA-13440, 1999.
4. Tabata, T., "Backscattering of Electrons from 3.2 to 14 MeV," Phys. Rev. 162, pp 336-347, 1967.

Appendix A: MCNP5 Input File

```
Ebert: 6.0-10.2 MeV electrons on 4.85 g/cm2 Ag
c*****************************************************************
c By Phuongloan Libby-University of New Mexico                    *
c Input File B.5: Sample input template for Ebert, transmission and backscatter  *
c These input files and associated output files are located on cfs in  *
c  /x6code/benchmarks/electron/ebert/ebert.ag.tar,ebert.c.tar,ebert.u.tar, and  *
c  bert.back.tar                                                  *
c This input file is based on silver simulations.                 *
c The changes needed for carbon and uranium are indicated in italics.  *
c *****************************************************************
1  1   -10.48  -1    2   -3
c Carbon
c 1  1    -1.7/-2.0/-2.267 -1  2  -3
c Uranium
c 1  1    -19.0    -1 2  -3
2  0            10  -11  -14
3  0           -12   13  -14
4  0          -999   #1   #2   #3
5  0           999

1     pz  0.0     $ target
2     pz  -0.46279  $ change surface 2 to alter thickness
3     cz  1.0
10    pz -10.     $ tally surfaces
11    pz  -9.99
12    pz  10.
13    pz  9.99
14    cz  12.
100   pz -11
999   so 100

mode p e
imp:p,e 1 3r 0
phys:e 10.2 8j
sdef par=3 sur=100 pos=0 0 -11. vec=0 0 1 dir=1 rad=d1 erg=10.2
si1 0.3
fc1 backscatter - use first cos bin
f1:e 2
tf1 5j 1 2j
fc31 transmission target face - 2nd bin
f31:e 1
fc41 transmission top - 2nd bin
f41:e 3
```

```
c0 0 1
fq0 f c
m1 47000 1
c       [carbon] m1 6000 1
c       [uranium] m1 92000 1
print
prdmp 2j 1 1
nps 1.5e6
rand hist=1 stride=152917777
```

Appendix B: MCNP4B Input File

```
Ebert - 10.2 MeV electrons on 4.85 g/cm2 Ag
c Sample input template for Ebert, transmission and backscatter. These input files and
c associated output files are located on cfs in
c /x6code/benchmarks/electron/ebert/ebert.ag.tar,ebert.c.tar,ebert.u.tar, and ebert.back.tar.
c This input file is based on silver simulations. The changes needed for carbon and
c uranium are indicated in italics.
1 1   -10.48  -1   2   -3
2 0           10 -11 -14
3 0          -12  13 -14
4 0         -999  #1  #2  #3
5 0          999

1     pz  0.0              $ target
2     pz -0.46279          $ change surface 2 to alter thickness
3     cz  1.0
10    pz -10.              $ tally surfaces
11    pz -9.99
12    pz  10.
13    pz  9.99
14    cz  12.
100   pz -11
999   so 100

mode p e
imp:p,e 1 3r 0
phys:e 10.2 8j
sdef par=3 sur=100 pos=0 0 -11. vec=0 0 1 dir=1 rad=d1 erg=10.2
si1 0.3
fc1 backscatter - use first cos bin
f1:e 2
tf1 5j 1 2j
fc31 transmission target face - 2nd bin
f31:e 1
fc41 transmission top - 2nd bin
f41:e 3
c0 0 1
fq0 f c
m1 47000 1
c       [carbon] m1 6000 1
c       [uranium] m1 92000 1
print
prdmp 2j 1 1
nps 10000
```