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COMPUTATION OF THE TOTAL SCATTERING CROSS SECTIONS FOR THE METALLOIDS

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ABSTRACT
Total Cross-Sections (TCS) of elastic electron-atom scattering for the metalloids Boron (B), Silicon (Si), Germanium (Ge), Arsenic (As), Antimony (Sb), Tellurium (Te) and Polonium (Po). The computed TCS were calculated using Born, Eikonal and the Optical Theorem approximation methods with the Lenz-Jensen potential, at electron incident energies between 1 to 1000 eV.

Keywords: Cross Section, Scattering, Metalloids, Optical theorem, Born approximation, Eikonal approximation

INTRODUCTION

Electron-atom and electron-molecule collision processes play an important role in many systems such as solar plasmas, aurorae, discharge or electron-beam lasers, plasma processing devices, etc. According to Tanaka and Inokuti (2000) electron collisions with molecules initiate the first step in plasma generation.

In scattering theory, the Total Cross-Section (TCS) is a measure of the probability that an interaction occurs; the larger the cross section, the greater the probability that an interaction will take place when a particle is incident on a target (Abdu, 2018a; Abdu, 2018b; Anchaver, 2003).

Elastic electron-atom scattering takes place if the final state of an atom after the interaction coincides with the initial one (Winitzki, 2004). Total and differential cross-sections for such a process can be calculated in various approximations — Born (Merzbacher, 1970)), Eikonal (Innanen, 2010; Shajesh, 2010), optical theorem (Lokajicek & Kundrat, 2009; Ronniger, 2006), partial wave method (Cox & Bonham, 1967), etc. In this work, the total cross-sections of the metalloids (Halka & Nordstrom, 2010) Boron (B), Silicon (Si), Germanium (Ge), Arsenic (As), Antimony (Sb), Tellurium (Te) and Polonium (Po) were computed using the Born, Eikonal and Optical Theorem approximation methods.

Metalloids and their compounds are used in alloys, biological agents, catalysts, flame retardants, glasses, optical storage and optoelectronics, pyrotechnics, semiconductors, and electronics. Some uses of metalloids include: amorphous Boron is used as a rocket fuel igniter and in pyrotechnic flares with a distinctive green colour; Silicon is used extensively as a semiconductor in solid state devices in the computer and microelectronics industries; Germanium is used as a semiconductor in transistors and integrated circuits, as an alloying agent, as a catalyst, and also used in infrared spectroscopes and infrared detectors; Arsenic is used a doping agent in semiconductors for solid state devices, in bronzing, pyrotechnics, in making special glass and to preserve wood; Antimony alloys and compounds are used in batteries, low friction metals, cable sheathing, flame-proofing materials, paints, ceramic enamels, glass, etc; Tellurium is used make blasting caps, added to cast iron, in ceramics, etc; Polonium can be used as a short term atomic heat source, used in anti-static brushes to eliminate dust on photographic film, sealed in brushes to control radioactive emissions.

MATERIALS AND METHODS

We used the FORTRAN code program developed by Koonin & Meredith (1989) which takes the relativistic differential cross-section as a sum of squared modules of the real and imaginary scattering amplitudes. The amplitudes can be calculated through the phase shifts of spherical waves, which are obtained by integration of equations for radial wave functions. In these computations the analytical approximation for the atomic electrostatic potential given by Lenz and Jensen, called the Lenz-Jensen potential (Blister & Hautala, 1978), based on the Thomas-Fermi model, is used.

Scattering Theory

For particles of mass m and energy

$$E = \frac{\hbar^2 k^2}{2m} > 0 \qquad (1)$$

scattering from a central potential, V(r) is described by a wave function, ψ(r) that satisfies the Schrodinger Wave Equation (SWE)

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \qquad (2)$$

with the boundary condition at large distance

$$\psi_{r\to\infty} \to e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \quad (3)$$

Equation (3) holds for a beam of electrons incident along z-axis, and the scattering angle, θ is the angle between r and $\hat{z}$ while f is the complex scattering amplitude, which is the basic function we seek to determine (Babaji, Abdu & Taura, 2012). The differential cross-section is given by:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \quad (4)$$

The total cross-section is

$$\sigma = \int d\Omega \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = 2\pi \int_0^{\pi} \mathrm{d}\theta \sin\theta |f(\theta)|^2 \quad (5)$$

f is a function of both E and θ (Koonin & Meredith, 1989).

Approximation Methods

Approximations play a very important role in our understanding of processes that cannot be solved exactly. The calculation of scattering cross sections is one of the most important uses of Fermi's Golden Rule (Wacker, 2011). Fermi's rule involves only one matrix element of the interaction which makes it a first order approximation to the exact result. This approximation suggests an approximation to the complex scattering amplitude. The Born approximation involves an approximation to the complex scattering amplitude (Merzbacher, 1970). It has been extensively used to study low energy as well as high energy scattering processes. The Eikonal approximation is a technique for estimating the high energy behaviour of a forward scattering amplitude (Innanen, 2010). It was originally developed for potential scattering in quantum mechanics, where one approximates the classical trajectory corresponding to forward scattering by a straight line and uses a WKB approximation for the wavefunction (Sakuri, 1985). The optical theorem relates the forward scattering amplitude to the cross section (Lokajicek & Kundrat, 2009).

The Lenz-Jensen Potential

One practical application of the theory discussed above is the calculation of the scattering of electrons from neutral atoms. In general this is a complicated multi-channel scattering problem since there can be reactions leading to final states in which the atom is excited. However, as the reaction probabilities are small in comparison to elastic scattering, for many purposes the problem can be modeled by the scattering of an electron from a central potential (Koonin & Meredith, 1989). This potential represents the combined influence of the attraction of the central nuclear charge (Z) and the screening of this attraction by the Z atomic electrons. For a neutral target atom, the potential vanishes at large distances faster than r^{-1}**.** A very accurate approximation to this potential can be had by solving for the self-consistent Hartree-Fock potential of the neutral atom. However, a much simpler estimate can be obtained using an approximation to the Thomas-Fermi model of the atom given by Lenz and Jensen (Blister & Hautala, 1978)

$$V = -\frac{Ze^2}{r}e^{-x}(1 + x + b_2x^2 + b_3x^3 + b_4x^4); \quad (6)$$

with

$e^2 = 14.409;\ b_2 = 0.3344;\ b_3 = 0.0485;\ b_4 = 2.647 \times 10^{-3};$

and

$$x = 4.5397Z^{\frac{1}{6}}r^{\frac{1}{2}} \quad (7)$$

This potential is singular at the origin. If the potential is regularized by taking it to be a constant within some small radius r_{min} (say the radius of the atom's 1s shell), then the calculated cross-section will be unaffected except at momentum transfers large enough so that $qr_{min} \gg 1$.

The incident particle is assumed to have the mass of the electron, and, as is appropriate for atomic systems, all lengths are measured in angstrom (Å) and all energies in electronvolt (eV). The potential is assumed to vanish beyond 2Å. Furthermore, the r^{-1} singularity in the potential is cutoff inside the radius of the 1s shell of the target atom.

Research Methodology

A FORTRAN program developed by Koonin & Meredith (1989) was the main program used for all the computations. The program is made up of four categories of files: common utility programs, physics source code, data files and include files. The physics source code is the main source code which contains the routine for the actual computations. The data files contain data to be read into the main program at run-time and have the extension .DAT.

The first thing done was the successful installation of the FORTRAN codes in the computer. This requires familiarity with the computer's operating system, the FORTRAN compiler, linker, editor, and the graphics package to be used in plotting.

The program runs interactively. The main menu below is displayed:

1. Change physical parameter
2. Change numerical parameters
3. Change output parameters
4. Display physical and numerical parameters
5. Display output parameters
6. Run the program
7. Stop the program

We made a menu choice of (1) and the following options were displayed:

1. Lenz-jensen potential: electron and neutral atom
2. Square well
3. Gausian well

We made a menu choice of (1) and it then displayed "Enter charge of the atomic nucleus" where we entered the nuclear charge (atomic number) of the first metalloid. It then displayed "Enter energy <ev>" where we entered the incident energy (1.0 eV) for the electron. It then displayed the numerical parameter which is the quadrature point with default value of 20 which we accepted. We then chose to display text output on the screen and save a copy. We then returned to the main menu and chose to run the program. This procedure is repeated for all the metalloids with various electron incident energies.

RESULTS AND DISCUSSION

Results were generated for several electron incident energies as presented in tables 1-3 below and plotted as given in figures 1-7:

Table 1: Computed Total Cross-Sections for Elastic Electron- Atom Scattering for B, Si, Ge, As, Sb, Te and Po using the Born Approximation Method with the Lenz-Jensen Potential.

Energy (eV)	TOTAL CROSS SECTION (Å^2)						
	B	Si	Ge	As	Sb	Te	Po
1.0	87.000	232.800	464.600	476.100	668.600	678.600	973.400
5.0	50.790	153.900	338.200	347.800	512.400	521.100	784.400
10.0	32.330	107.300	253.500	261.400	399.900	407.400	638.200
20.0	18.910	68.110	172.700	178.600	284.100	289.900	474.400
30.0	13.460	50.440	132.500	137.200	222.900	227.700	382.100
40.0	10.430	40.110	107.900	111.800	184.200	188.300	321.300
50.0	8.511	33.340	91.130	94.510	157.300	160.900	278.000
60.0	7.195	28.560	79.010	81.990	137.500	140.700	245.500
70.0	6.230	24.990	69.800	72.460	122.300	125.100	220.000
80.0	5.491	22.220	62.530	64.930	110.100	112.700	199.400
90.0	4.907	20.000	56.650	58.840	100.200	102.600	182.500
100.0	4.435	18.190	51.790	53.810	91.990	90.200	168.300
200.0	2.256	9.566	28.010	29.130	50.760	52.030	95.350
300.0	1.510	6.493	19.230	20.010	35.150	36.040	66.810
400.0	1.134	4.915	14.650	15.250	26.910	27.600	51.480
500.0	90.720	3.953	11.830	12.320	21.800	22.360	41.910
600.0	75.610	3.306	9.923	10.330	18.330	18.800	35.340
700.0	64.810	2.841	8.545	8.899	15.810	16.220	30.560
800.0	56.710	2.491	7.503	7.815	13.900	14.260	26.950
900.0	50.410	2.217	6.688	6.966	12.400	12.720	24.060
1000.0	45.370	1.998	6.032	6.283	11.190	11.490	21.750

From table 1 and figures 1-7, using the Born method, the calculated TCS are significantly higher than those obtained using the two other approximation methods. This is in agreement with Babaji *et al.* (2012). This is as a result of the fact that the Born approximation is only valid at high electron incident energies (Babaji *et al*., 2012). As observed, the calculated TCS of all the metalloids decrease with increasing incident energies from 1 to 1000 eV except those for Boron (fig. 1) which reduced to its minimum, 1.134 Å^2 at 400 eV, and then rose sharply to 90.720 Å^2 at 500 eV. Thereafter it continued to decrease with increasing electron incident energy. Also, the calculated TCS increased with increasing atomic number (Z) for the metalloids except for Boron between 500 – 1000 eV.

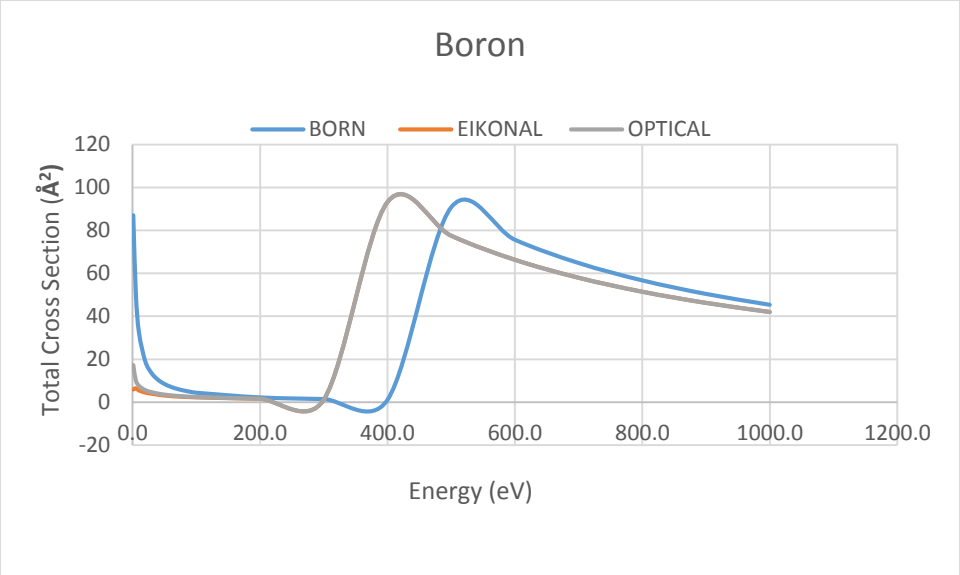

Fig 1: TCS for Boron using Born, Eikonal and Optical Theorem approximations

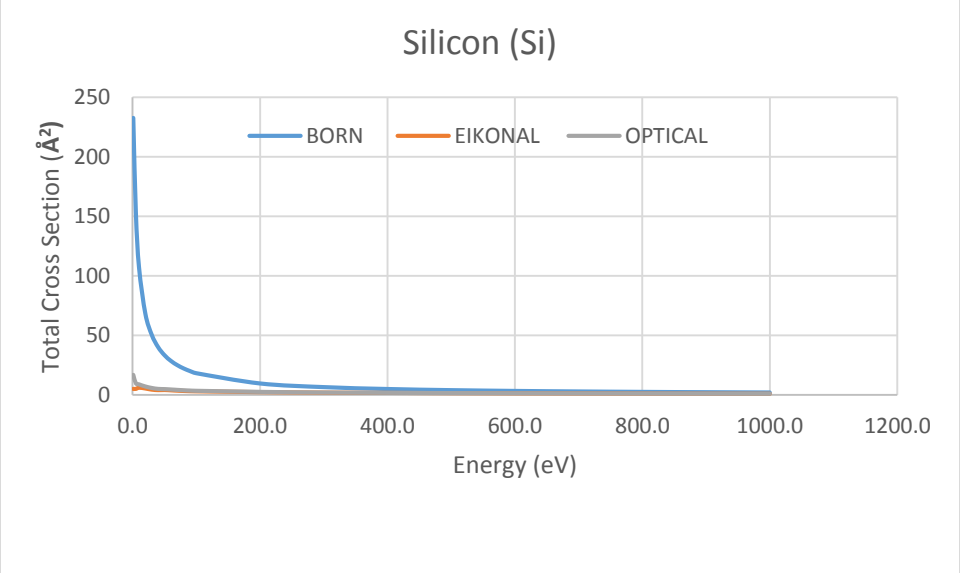

Fig. 2: TCS for Silicon using Born, Eikonal and Optical Theorem approximations

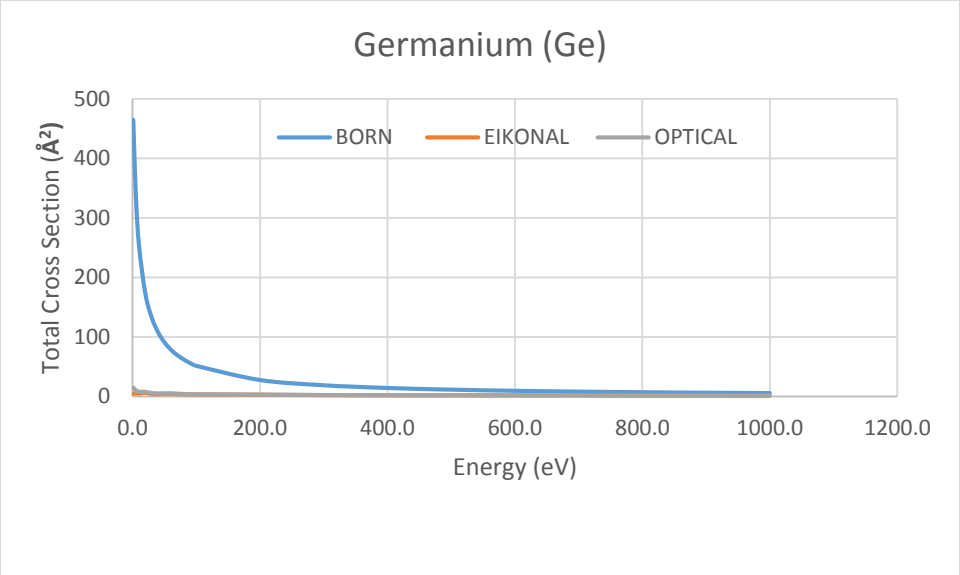

Fig. 3: TCS for Germanium using Born, Eikonal and Optical Theorem approximations

Table 2: Computed Total Cross-Sections for Elastic Electron- Atom Scattering for B, Si, Ge, As, Sb, Te and Po using the Eikonal Approximation Method with the Lenz-Jensen Potential.

Energy (eV)	TOTAL CROSS SECTION (Å²)						
	B	Si	Ge	As	Sb	Te	Po
1.0	5.895	5.212	4.825	4.863	4.649	4.763	4.838
5.0	6.423	5.209	5.363	4.818	5.054	4.902	3.372
10.0	5.465	6.173	4.884	5.085	6.909	7.302	5.555
20.0	4.449	5.547	6.169	6.224	4.367	4.182	3.171
30.0	3.935	4.567	4.351	4.422	5.618	5.388	4.173
40.0	3.465	4.152	4.134	4.079	4.112	4.170	4.856
50.0	3.093	4.258	4.569	4.370	3.750	3.680	4.445
60.0	2.823	3.973	4.537	4.593	3.577	3.575	3.904
70.0	2.624	3.675	4.055	4.135	3.707	3.626	3.233
80.0	2.471	3.429	3.690	3.743	3.814	3.800	3.018
90.0	2.346	3.254	3.501	3.522	3.914	3.877	3.066
100.0	2.237	3.145	3.352	3.366	3.940	3.917	3.299
200.0	1.540	2.438	3.066	3.084	2.758	2.746	3.113
300.0	1.163	2.018	2.436	2.459	2.739	2.729	2.384
400.0	93.090	1.766	2.182	2.184	2.581	2.587	2.502
500.0	77.470	1.572	2.071	2.068	2.210	2.245	2.319
600.0	66.290	1.418	1.978	1.986	1.989	1.995	2.302
700.0	57.920	1.296	1.864	1.882	1.919	1.920	2.241
800.0	51.410	1.197	1.736	1.762	1.853	1.859	2.171
900.0	46.220	1.114	1.615	1.642	1.782	1.787	2.060
1000.0	41.980	1.045	1.514	1.538	1.738	1.732	1.889

From table 2 and figures 1-7, using the Eikonal method, the TCS for the metalloids are significantly lower than those calculated using the other two methods. All the calculated TCS decreased with increase in electron incident energies except for those of Boron (Fig. 1) that reached a minimum of 1.163 Å^2 at 300 eV and rose sharply to 93.090 Å^2 at 400 eV.

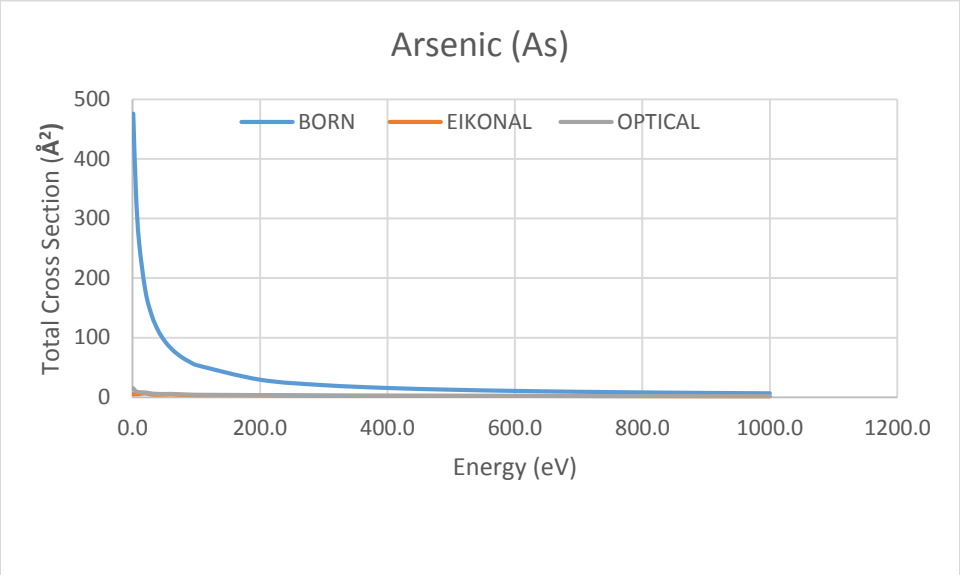

Fig 4: TCS for Arsenic using Born, Eikonal and Optical Theorem approximations

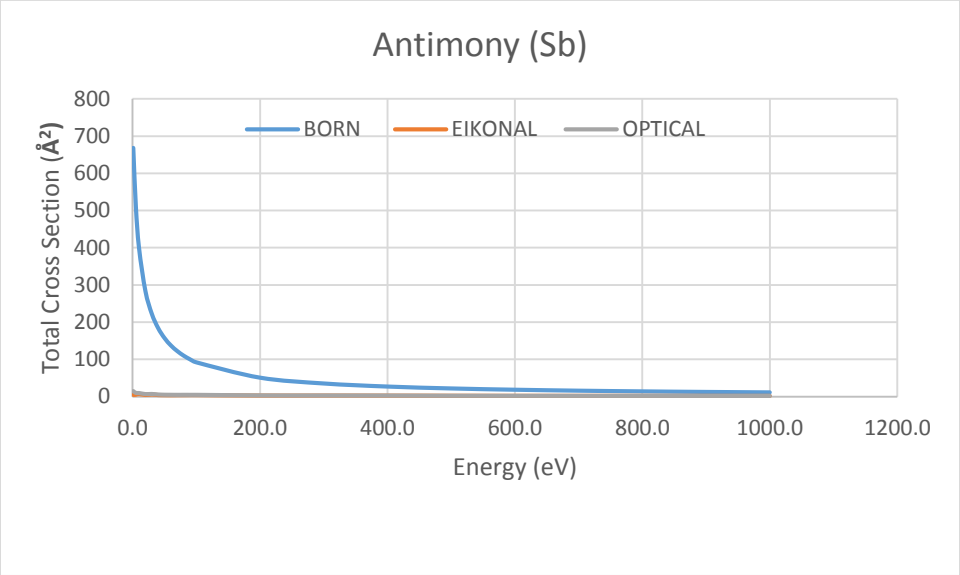

Fig. 5: TCS for Antimony using Born, Eikonal and Optical Theorem approximations

Table 3: Computed Total Cross-Sections for Elastic Electron- Atom Scattering for B, Si, Ge, As, Sb, Te and Po using the Optical Theorem with the Lenz-Jensen Potential.

Energy (eV)	TOTAL CROSS SECTION (Å^2)						
	B	Si	Ge	As	Sb	Te	Po
1.0	17.280	16.990	15.210	15.310	14.620	14.620	1.551
5.0	10.130	9.930	10.610	10.150	9.776	9.686	7.781
10.0	7.580	8.975	8.283	8.402	9.493	9.740	8.762
20.0	5.564	7.183	7.966	7.997	6.653	6.525	5.530
30.0	4.647	5.950	6.123	6.174	7.023	6.887	6.188
40.0	3.996	5.153	5.470	5.443	5.616	5.671	6.204
50.0	3.524	4.990	5.455	5.333	4.915	4.839	5.718
60.0	3.179	4.674	5.476	5.491	4.804	4.817	5.122
70.0	2.918	4.331	4.972	5.070	4.627	4.575	4.110
80.0	2.710	4.021	4.475	4.535	4.702	4.691	3.899
90.0	2.540	3.763	4.242	4.250	4.685	4.653	4.015
100.0	2.395	3.568	4.021	4.057	4.656	4.636	4.165
200.0	1.567	2.663	3.406	3.434	3.228	3.225	3.705
300.0	1.170	2.127	2.651	2.670	3.016	3.005	2.604
400.0	93.310	1.840	2.345	2.350	2.777	2.797	2.656
500.0	77.550	1.634	2.205	2.203	2.333	2.367	2.530
600.0	66.330	1.471	2.073	2.085	2.104	2.107	2.509
700.0	57.940	1.339	1.920	1.945	1.998	1.997	2.386
800.0	51.430	1.231	1.771	1.800	1.919	1.920	2.225
900.0	46.230	1.142	1.645	1.672	1.855	1.855	2.050
1000.0	41.990	1.066	1.546	1.567	1.810	1.806	1.867

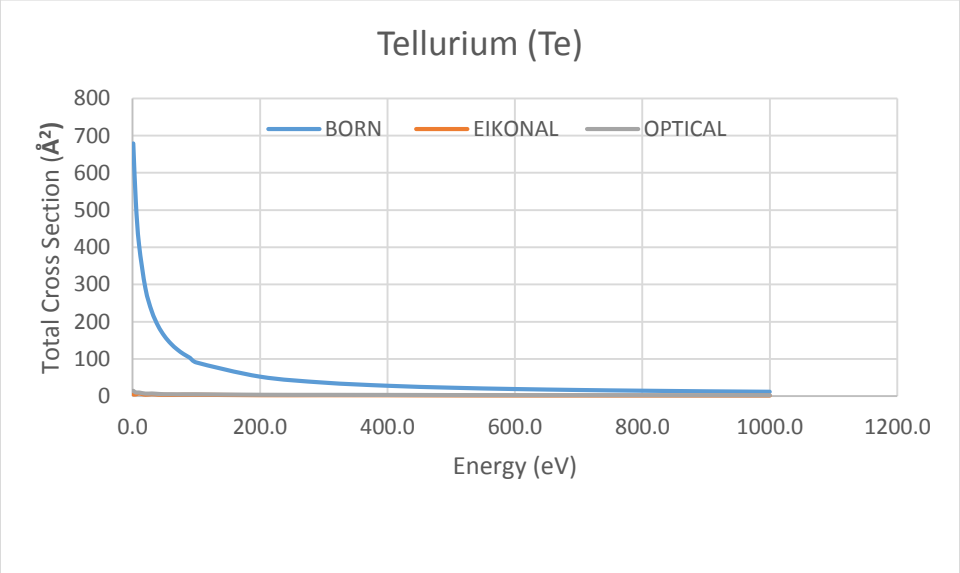

Fig. 6: TCS for Tellurium using Born, Eikonal and Optical Theorem approximations

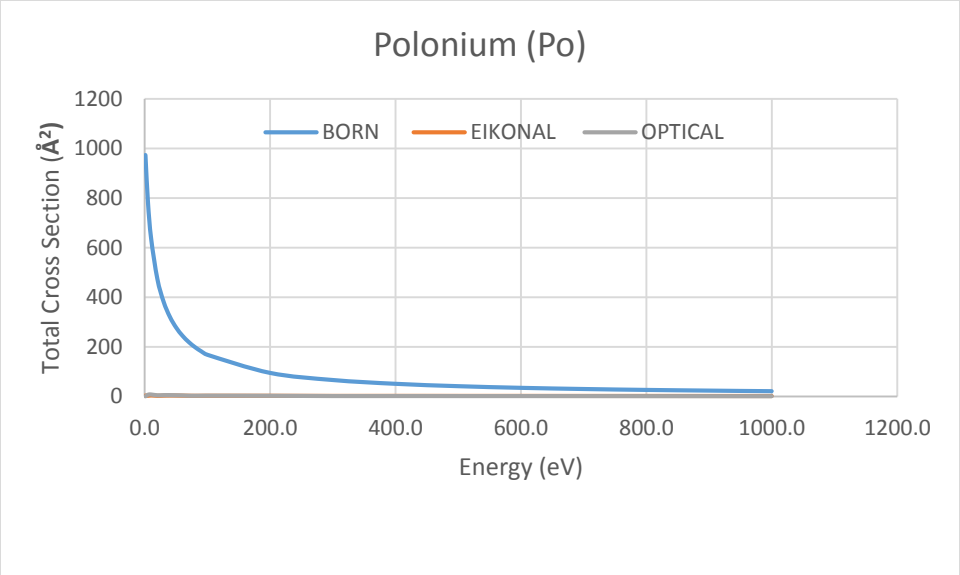

Fig. 7: TCS for Polonium using Born, Eikonal and Optical Theorem approximations

From table 3 and Figures 2-6, using the Optical theorem method, the calculated TCS for Si, Ge, As, Sb and Te decrease with increasing incident energy between 1 to 1000 eV. Those for Po (Fig. 7) fluctuated in the energy range of 1 to 400 eV, then decrease with increasing incident energy between 400 to 1000 eV. The TCS for B (Fig.1) decreased to a minimum of 1.170 $Å^2$ at 300 eV, then rose sharply to 93.310 $Å^2$ at 400 eV, and thereafter decreased with increasing incident energy between 400 to 1000 eV.

The calculated TCS using Eikonal and Optical theorem approximation methods are in good agreement with the TCS calculated by Cox and Bonham (1967). However TCS calculated using the Born approximation method are much higher than the values for the energy range considered. This is because the Born approximation is only valid at high electron incident energies (Babaji *et al.*, 2012).

CONCLUSION

Computed Total Cross-Sections (TCS) of elastic electron-atom scattering for the metalloids were computed using the Born, Eikonal and the Optical theorem approximation methods with the Lenz-Jensen potential, at incident energies of 1 to 1000 eV. Results obtained using the Eikonal and Optical theorem methods are in good agreement with the experimental TCS values of NIST SRD 64 (2016).

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