Acta Scientifica Balcanica, 2021, 2(1)

DOI:10.7251/ASB2102011K **UDC: 544.174.2:539.124-16**

Original scientific paper

COMPARING CALCULATED VALUES OF ELECTRON MEAN ENERGY OBTAINED THROUGH DIFFERENT SETS OF CROSS SECTIONS FOR e^-/Ar INTERACTION

Danijela Kuzmanović[1], Snježana Dupljanin[2*]

[1]*University of Ljubljana, Faculty of Mathematics and Physics, 19 Jadranska Street, 1000 Ljubljana, Slovenia*
[2*]*University of Banja Luka, Faculty of Natural Sciences and Mathematics, Mladena Stojanovića 2, 78000 Banja Luka, the Republic of Srpska, Bosnia and Herzegovina*
***Corresponding Author:** snjezana.dupljanin@pmf.unibl.org

Summary

The paper presents analysis of existing data on cross sections for electrons scattering on Argon atoms, using the LXCat database. We compared results acquired by different groups of researchers, i.e. different databases: Hayashi, Triniti, Morgan and BSR bases. Using Bolsig+ code, values of mean energy of electrons' swarm were calculated and compliance analysis of calculated values for different considered sets of cross sections as entry parameters was performed.

Key words: cross sections, mean energy, databases

INTRODUCTION

Physics of ionized gases is an empiric discipline dealing with researching interactions between bearers of electricity and gasses' constituents. Some examples of consequences of that interaction in nature are lightning and polar light. This discipline of physics found its application in semiconductor industry and production of integrated circuits, development of plasma screens, gas lasers, light sources, biophysics and medicine (Laroussi, 2020). More recently, electrical discharge is used to decrease or remove damaging gases from the atmosphere, such as carbon dioxide, methane, nitrogen oxides, primarily by means of dielectric barrier and impulse corona discharge (Bie *et al*., 2011; Zhou *et al*., 2017). Rapid technological development both enables and demands intensifying research in this field. To that regard, a need for plasma models as an indispensable tool for the purpose emerged. The need for models was triggered due to the non-economical nature of empirical technological procedures, that is, complexity of devices used, enabling a detailed insight to physical nature of the process, and for helping in understanding various kinetic phenomena. Entry data for all plasma models are sets of cross sections and transport coefficients (mean energy, drift velocity, etc.) in as wide as possible range of mean energy of electrons.

The subject of research in this paper is Argon (Ar), which, from the standpoint of electrical discharge, has been studied for over 100 years. With discovery of a minimum in an elastic cross section on low electron energies by Ramsauer, Townsend and Baily, Argon became a focal point of intense studies. Easy accessibility of the gas and successful clarification of effects applying quantum mechanics evoked further research (Raju, 2006).

The goal of this work is to analyze existing data on electron scattering cross section in Argon, using the LXCat database (Triniti database), compare results acquired by different groups of researchers and look if there is compliance of calculated transport coefficients (electrons mean energy) for different considered sets of cross sections.

MATERIAL AND METHODS

The sets of cross sections for e^-/Ar interaction were taken from the LXCat database (https://fr.lxcat.net). This database was formed in 2010 and is open for collecting, presenting and transferring electron and ionic scattering cross sections, transport and rate coefficients, electron energy distribution functions and other data necessary for modeling low temperature plasma. In this work we have taken, compared and discussed cross sections for e^-/Ar interaction from several different databases: Hayashi, Triniti, Morgan and BSR base.

The calculation of a mean energy of the swarm of electrons moving in Argon under the effect of an external electric field was made using Bolsig+ code (Hagelaar i Pitchford, 2005; BOLSIG+) that is based on a solution of the Boltzmann equation in two term approximation (Boltzmann, 1872). Boltzmann's equation describes statistical behavior of a thermodynamic system that is not in thermodynamic balance. It is derived from general kinetic equations and has the following form:

$$\{\partial_t + \vec{v}\partial_{\vec{r}} + \vec{a}\partial_{\vec{v}}\}f(\vec{r},\vec{v},t) = -Jf(\vec{r},\vec{v},t), \quad (1)$$

where: $\vec{a} = \frac{e}{m}\left(\vec{E} + \vec{v}\times\vec{B}\right)$ – electron acceleration in electromagnetic field, f – imbalance distribution function and J – collision integral that contains information on numerous collision processes thus causing difficulties in solving the Boltzmann equation. A simplified form of this integral is given in an equation:

$$J(f) = \sum_{i,j} \int \left[f(\vec{v})F_i(\vec{V}) - f(\vec{v'})F_j(\vec{V}')\right]\vec{u}\sigma(ij,u,\Omega)d\vec{u'}d\vec{V}', \quad (2)$$

where f is a function of distribution of electrons, F is a function of distribution of gas particles, u is a velocity of relative movement, σ are differential elastic and inelastic cross sections, while the mark (') is used for factors after the impact. Further simplification of the Boltzmann equation is achieved under hydro-dynamic conditions enabling separation of kinetic equations to a velocity and spatial-time portion (Dupljanin, 2016). By solving the Boltzmann equation in two term approximation, it is possible to get the electron energy distribution function, and with certain mathematical procedures also the transport coefficients. Calculations were made for a number of values of reduced electric field (E/N), from 0.1 to 1000 Td ($1\ Td = 10^{-21}\ Vm^2$).

RESULTS AND DISCUSSION

Figure 1 (a and b) displays the cross sections for e$^-$/Ar interaction taken from Hayashi and Triniti database, which are a part of the LXCat base (Hayashi and Triniti database).

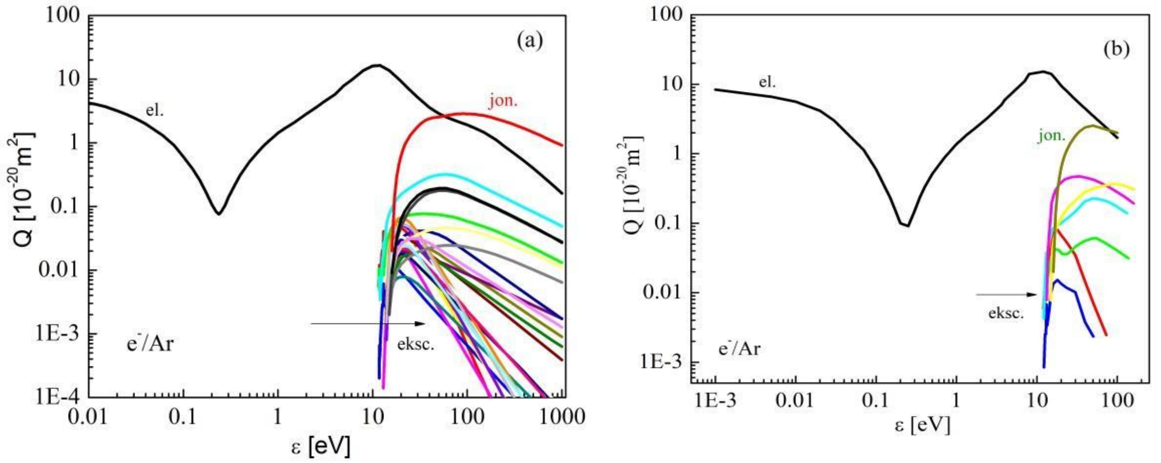

Figure 1. The cross sections for e$^-$/Ar interaction taken from: (a) Hayashi database (Hayashi database), (b) Triniti database (Triniti database)

The Hayashi set of cross sections consists of 27 cross sections, of which 1 elastic, 25 excitation and 1 ionization cross sections. Triniti set of cross sections includes 1 elastic, 6 excitation and one ionizing cross section.

Figure 2 (a and b) displays the cross sections for e$^-$/Ar interaction taken from Morgan's and BSR database (Morgan and BSR database). Morgan's set consists of 4 cross sections, of which 1 elastic, 1 ionizing and 2 excitation cross sections, while the BSR set includes 1 elastic, 1 ionizing and 13 excitation cross sections.

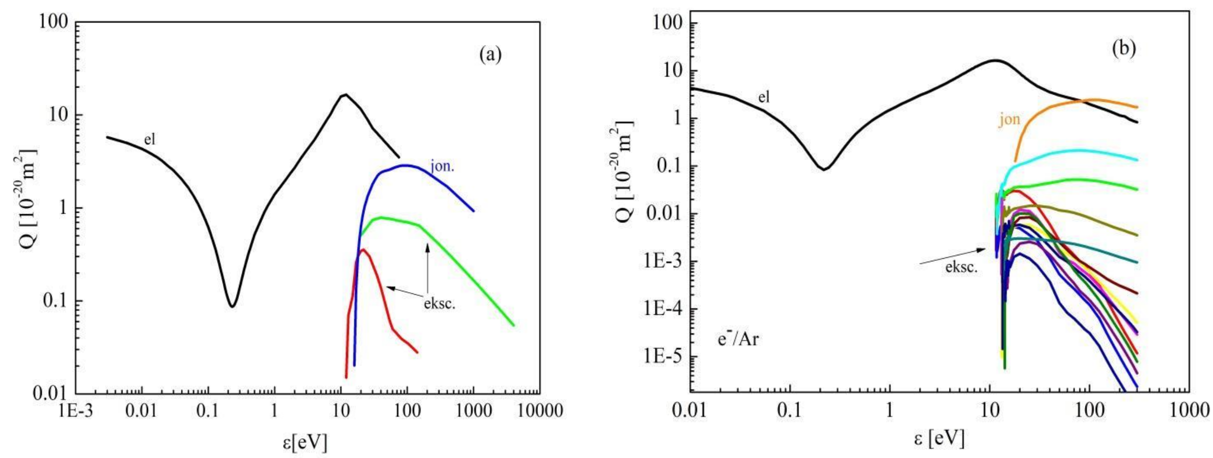

Figure 2. The cross sections for e$^-$/Ar interaction taken from: (a) Morgan's database (Morgan database), (b) BSR database (BSR database)

By comparing the cross sections displayed on Figure 1 and 2, we observe certain discrepancies in values for certain types of cross sections, primarily for excitation cross sections.

Figure 3 (a) displays comparison of dependence of excitation cross sections to level $1s_5$ in Ar, from electron energy ranging from 10 to 500 eV. We compared data from databases Hayashi, Triniti, BSR and Morgan. In Figure 3 we can see that results from all four databases follow the same distribution (they have the same shape), noting that Morgan database results have a more significant deviation compared to other three databases.

Table 1 displays maximum values of excitation cross sections for each of the databases. Significant deviation (a whole order of magnitude) of maximum excitation cross section for data from the Morgan database is registered.

Figure 3 (b) displays comparison of dependence of excitation cross sections to a level $1s_4$ in Ar, from electron energy ranging from 11-1100 eV, from databases Triniti, Hayashi and BSR. The Morgan database does not contain data for this process. As we can see in the Figure, excitation cross sections from Hayashi and BSR databases have very good accordance in the whole energy range. It can also be observed that in the range 11-16 eV cross sections of Triniti database match with cross sections of the other two bases, while in the range 16-50 eV there is a prominent local minimum (σ_{min}=3.52·10^{-22} m^2) for approximately same energy (21.7eV) where cross sections of the other two databases have maximum (σ_{max}=7.57·10^{-22} m^2). The maximum excitation cross section of Triniti database is 6.24·10^{-22} m^2 for an energy level of 53.57 eV.

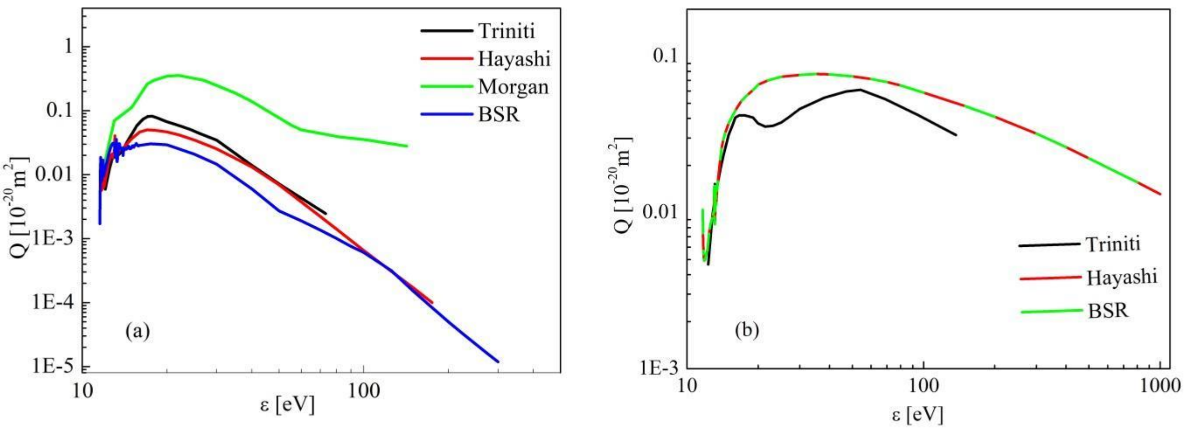

Figure 3. (a) Comparing dependence of excitation cross section to level $1s_5$ in Ar from electron energy for four different databases (Triniti, Hayashi, Morgan, BSR); (b) Comparing dependence of excitation cross section to level $1s_4$ in Ar from electron energy for three different databases (Triniti, Hayashi, BSR)

Table 1. Maximum values of excitation cross section to level $1s_5$ in Ar for four databases

Database	ε [eV]	σ_{max} [10^{-22} m^2]
BSR	13.21	3.55
HAYASHI	17.34	5.01
TRINITI	17.27	8.30
MORGAN	21.47	35.80

Calculation of mean energy of electrons moving in Ar under the effect of external electric field was made using Bolsig+ code in a wide range of E/N, while sets of cross sections from database Triniti, Hayashi, BSR and Morgan were used as entry data, presented and discussed afore. Calculation results are given in Table 2 and presented in Figure 4.

Table 2. Calculated values of electron mean energy depending on electric field, for four different sets of cross sections

E/N [Td]	Mean energy Triniti [eV]	Mean energy Hayashi [eV]	Mean energy BSR [eV]	Mean energy Morgan [eV]
0.100	0.789	0.781	0.751	0.788
0.127	0.883	0.874	0.839	0.882
0.160	0.990	0.979	0.939	0.991
0.203	1.113	1.097	1.054	1.113
0.257	1.252	1.230	1.185	1.251
0.326	1.407	1.380	1.335	1.406
0.413	1.580	1.548	1.503	1.580
0.522	1.772	1.737	1.693	1.777
0.661	1.980	1.948	1.904	1.998
0.838	2.209	2.180	2.138	2.245
1.061	2.461	2.434	2.397	2.519
1.343	2.742	2.712	2.683	2.823
1.701	3.058	3.019	2.998	3.159
2.154	3.409	3.361	3.348	3.531
2.728	3.800	3.743	3.738	3.940
3.455	4.234	4.172	4.173	4.383
4.375	4.672	4.611	4.606	4.795
5.541	5.007	4.953	4.927	5.074
7.017	5.210	5.161	5.110	5.221
8.886	5.340	5.292	5.219	5.305
11.250	5.440	5.395	5.308	5.370
14.250	5.550	5.494	5.396	5.438
18.050	5.653	5.602	5.499	5.517
22.850	5.763	5.720	5.622	5.612
28.940	5.852	5.849	5.770	5.727
36.650	5.996	5.991	5.946	5.865
46.420	6.214	6.145	6.152	6.029
58.780	6.343	6.314	6.392	6.221
74.440	6.569	6.501	6.662	6.441
94.270	6.790	6.711	6.970	6.690
119.400	7.030	6.954	7.323	6.975
151.200	7.318	7.236	7.735	7.297
191.400	7.682	7.573	8.230	7.669
242.400	8.134	7.987	8.844	8.108
307.000	8.712	8.508	9.625	8.641
388.800	9.463	9.178	10.640	9.305
492.400	10.490	10.060	12.000	10.150
623.600	11.940	11.250	13.820	11.260
789.700	14.090	12.860	16.250	12.720
1000.000	17.400	15.090	19.490	14.680

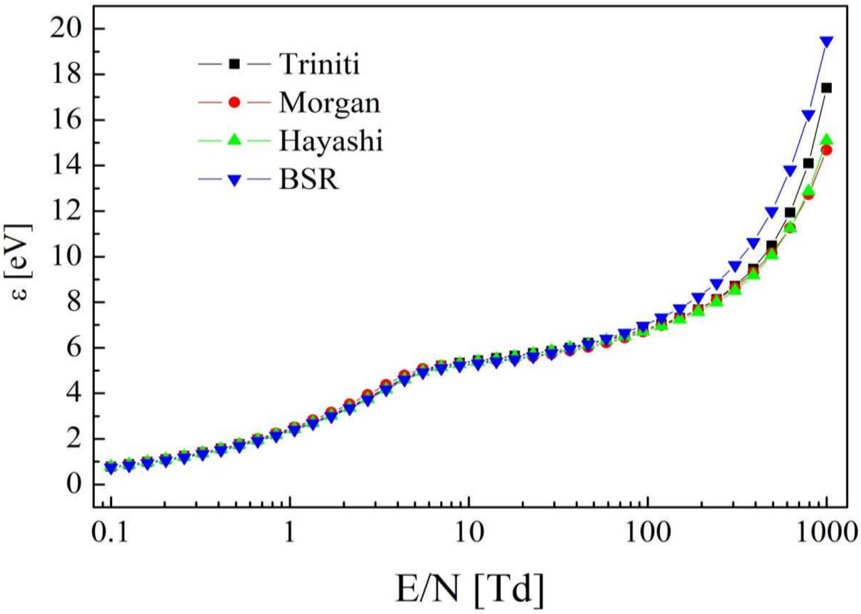

Figure 4. Comparing calculated values of electron mean energy as function of reduced electric field (E/N) for four different sets of cross sections

Figure 4 displays dependence of electron mean energy from reduced electric field in the range from 0.1 to 1000 Td, for four different sets of cross sections. Mean energy values calculated using Bolsig+ code with entry data of cross sections from Hayashi and Morgan databases agree very well in the whole range of E/N, as can clearly be seen in the Figure. The curve obtained from BSR database data follows the previous two curves from 0.1 to 100 Td, while in the range from 100 to 1000 Td there are minor deviations, up to 22%. Deviation of the curve obtained based on Triniti data is somewhat less than the BSR curve (maximum 13%) and starts from 774.2 Td.

CONCLUSION

The paper presents analysis of existing data on cross sections for electrons scattering on Argon atoms, using the LXCat database. We compared results derived from different databases and we analyzed the agreement between calculated values of mean energy of electrons moving in a neutral Argon gas under the effect of an external electric field, for different considered sets of cross sections. We analyzed four databases: Hayashi, Triniti, Morgan and BSR base.

The paper graphically displayed sets of cross sections and compared data from mentioned four databases for elastic, ionizing and excitation cross sections for $1s_5$ and $1s_4$ levels. Quite good matching is visible for elastic and ionizing cross sections. Data from all analyzed bases follow the same distribution (they have the same shape), and the deviations are not larger than 35%. Higher deviations were noticed in analyses of excitation cross sections where deviations go up to 50%.

Electron mean energy values calculated using BOLSIG+ code based on different sets of cross sections as entry parameters, in the range from 0.1 to 1000 Td, display a high level of matching for all analyzed databases. Maximum deviation of 22% appears in the range from 100 to 1000 Td, primarily due to significant difference in absolute values of excitation cross sections from different databases.

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Received 02 March 2022.
Accepted 07 April 2022.