Acta Scientifica Balcanica, 2021, 2(1)

DOI:10.7251/ASB2102027B **UDC:539.16.004.4:539.184.27**

Rewiev paper

CALCULATION OF REDUCED IONIZATION COEFFICIENT AND DEMONSTRATION OF OBTAINING CROSS SECTION SETS USING SWARM METHOD ON AN EXAMPLE OF NEON GAS

Dragana Budiša[1], Snježana Dupljanin[2*]

[1]*ProCredit Bank, Franca Lehara bb, 71000 Sarajevo, Bosnia and Herzegovina*
[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

This paper presents the use of swarm method for obtaining sets of cross sections on an example of Neon gas (Ne). Cross sections for e^-/Ne interaction available in the LxCat database were presented and discussed. The following three bases were selected: Biagi-v7.1, Morgan and Siglo. We used Bolsig+ code to calculate reduced ionization coefficient (α/N), after which calculated values were compared to measured values in the Dutton base. The swarm method was demonstrated in the α/N example, where the Morgan cross sections set was used as an entry parameter for calculation of coefficient.

Key words: swarm method, cross sections, databases

INTRODUCTION

Plasma is a natural phenomenon as more than 90% of the universe is in the state of plasma. On the other hand, plasma can be artificially made and as such it found its application in technology (e.g. plasma screens and light sources). For modification of biomaterial surfaces low temperature plasma is used, which is sometimes also called cold plasma. Its characteristic is low level of ionization at low or atmospheric pressure. Low temperature plasma has a wide spectrum of application, from medicine where it is used, inter alia, in stomatology, dermatology treatments and sterilization of medical equipment, to production and material processing in industry (Walschus *et al*, 2011).

One way to develop plasma technology is mathematical modeling of processes and interactions with different objects where it is crucial for the entry of parameters of plasma models. The need for modeling appeared due to non-economical and technically complex procedures related to processes of generating and applying the plasma itself. Entry parameters for such models are sets of cross sections and transport and rate coefficients (Dupljanin, 2016). One of the methods for obtaining cross sections is a swarm method (Dupljanin, 2016), which is presented in this paper on an example of neon gas.

Neon is a single atom gas for which experimental data are easily accessible. It is the fifth most common element in the universe, while in Earth's atmosphere it is present in a very low concentration. Its largest use is in the production of neon advertisements. In a vacuum tube for gas discharge, Neon emits red-orange color, while in fact only red lamps contain pure Neon. Medical treatments with Neon atmospheric plasma are very efficient for treating microorganisms, i.e. a large number of bacteria and fungi, even in 60 seconds intervals. The experiments showed that Neon plasma has positive effects of inactivation of gram negative and gram positive bacteria, human pathogens, pathogens in food and other microorganisms (Tanişli *et al*, 2016).

The goal of this work is to analyze existing data for cross sections from LXcat database on an example of reduced ionization coefficient for electrons that move in Neon gas under the effect of external electric field, and displaying swarm method as one of methods for obtaining sets of cross sections.

MATERIAL AND METHODS

Cross sections for e^-/Ne interaction were taken from LXCat database (https://fr.lxcat.net): Biagi-v7.1, Morgan and SIGLO. Using Bolsig+ code (Hagelaar and Pitchford, 2005; http://www.bolsig.laplace.univ-tlse.fr/), which is based on solution of Boltzmann equation in two term approximation (Boltzmann, 1872), we calculated reduced ionization coefficient (α/N) in a wide range of reduced electric field (E/N) ranging 1-1000 Td (1 Td = 10^{-21} Vm^2). The swarm method is presented on the basis of this coefficient.

Swarm method for determining cross sections comprises of several steps: measuring the parameters of electrons swarm – such as drift velocity, characteristic energy, ionization coefficient, etc; forming a starting set of cross sections for certain gas being researched; determining the electron energy distribution functions depending on E/N; calculating parameters of the swarm and their comparing with measured values of step one (Raju, 2006). Then the adjustment follows, i.e. modification of a starting set of cross sections and this procedure is repeated until there is a satisfying degree of compliance between the measured and calculated values of transport parameters. In this way, using this method gives us a complete set of cross sections, representing microscopic characteristics, and a set of transport coefficients, representing macroscopic characteristics of the researched gas. This set is very significant as it represents the entry parameter that ‘plasma modelers’ use during researching application of a certain type of low temperature plasma. The success of the method itself depends on entry data that need to be provided and on the accuracy of measurement and calculation of transport coefficient.

RESULTS AND DISCUSSION

Figure 1 displays a set of cross sections from Biagi-v7.1 database (Biagi-v7.1 database), depending on electrons energy, and it includes one elastic momentum transfer cross section, nine excitation cross sections and one ionizing cross section.

Figure 2 displays a set of cross sections from Morgan database (Morgan database), depending on electrons energy, and it includes one elastic momentum transfer cross section, two excitation cross sections and one ionizing cross section.

Figure 3 displays a set of cross sections from Morgan database (Siglo database), depending on electrons energy, and it includes one elastic momentum transfer cross section, two excitation cross sections and one ionizing cross section.

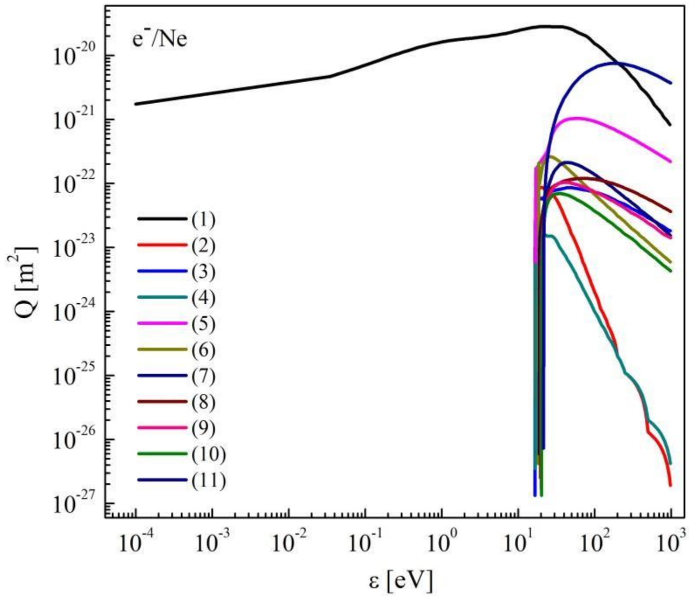

Figure 1. Set of cross sections for e-/Ne interaction (Biagi-v7.1 database): elastic momentum transfer cross section: (1); excitation cross sections: (2), (3), (4), (5), (6), (7), (8), (9) and (10); ionization cross section: (11)

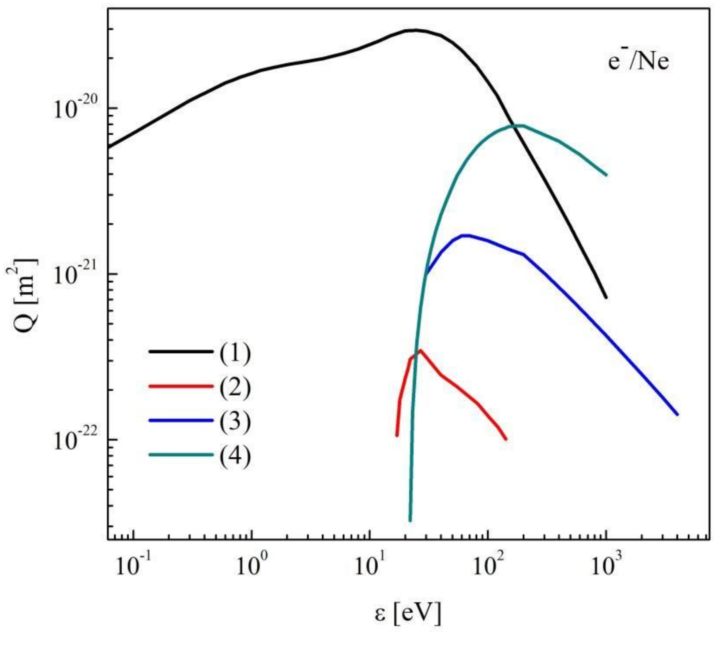

Figure 2. Set of cross sections for e-/Ne interaction (Morgan database): elastic momentum transfer cross section: (1); excitation cross sections: (2) and (3); ionization cross section: (4)

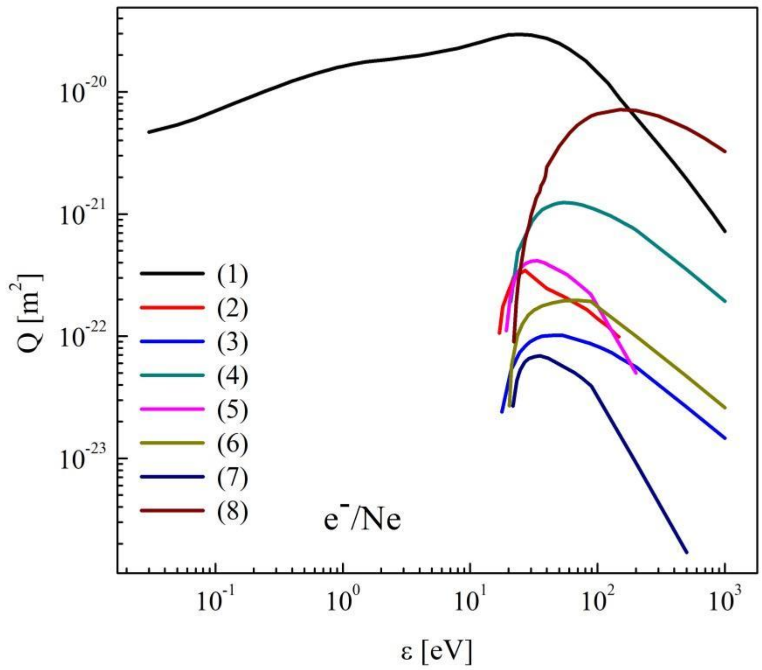

Figure 3. Set of cross sections for e$^-$/Ne interaction (Siglo database): elastic momentum transfer cross section: (1); excitation cross sections: (2), (3), (4), (5), (6) and (7); ionization cross section: (8)

To demonstrate the swarm method, we selected a set of cross sections from the Morgan database, shown in Figure 2. This set of cross sections includes the following processes:

(1) Elastic momentum transfer cross section: $e + Ne \rightarrow e + Ne$,

(2) Excitation cross section for metastable excitation: $e + Ne \rightarrow e + Ne^*$, with energy threshold $\varepsilon = 16.62\ eV$,

(3) Excitation cross section for total excitation: $e + Ne \rightarrow e + Ne^*$, with energy threshold $\varepsilon = 16.62\ eV$,

(4) Ionization cross section: $e + Ne \rightarrow e + e + Ne^+$ with energy threshold$\varepsilon = 21.56\ eV$.

Using Bolsig+ code, we calculated reduced ionization coefficient (α/N) in function of a reduced electric field (E/N) ranging 1-1000 Td with the Morgan set of cross sections as the entry parameter (Figure 2). Calculation results are presented with black line in Figure 4, where symbols are used to point to available experimental results in the Dutton database (Dutton database). We see that the compliance between calculated and measured values is satisfactory throughout the whole observed range of E/N.

Since Neon is a gas with reliable sets of cross sections in different databases, we shall present the swarm method by going "backwards", calculating α/N with three different modified Morgan sets of cross sections. Considering that ionization coefficient is most sensitive to electronic excitations, the first modification was made by excluding the excitation cross section: $e + Ne \rightarrow e + Ne^*$ with energy threshold ε=16.62 eV, that is, cross section for metastable excitation from the starting Morgan set (Figure 2). Result of those calculations is shown by the red line on Figure 5 and we can see that the degree of compliance between calculated and measured α/N values is significantly decreased everywhere, except for the highest values of E/N.

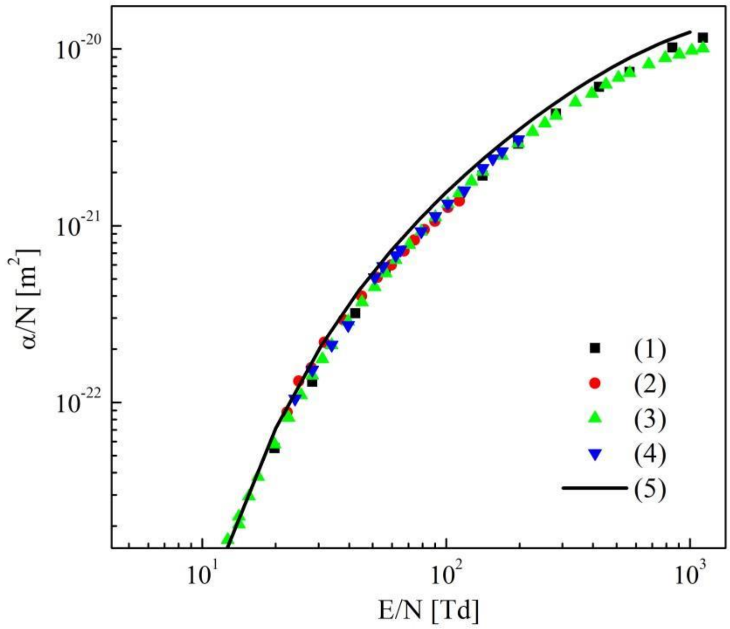

Figure 4. Reduced ionization coefficient (α/N) in function E/N for electrons in Ne gas: symbols (1), (2), (3) and (4) display measured values from Dutton database (Dutton database) while black line (5) shows calculated values using Bolsig+ code

The second modification was made excluding the second excitation cross section: $e + Ne \rightarrow e + Ne^{*}$, with energy threshold ε=16.62 eV, from the starting Morgan set (Figure 2), where we have total excitation. Result of calculating α/N with such a modified set as entry parameter is presented by the blue line in Figure 5. We see that excluding this excitation process leads to an additional decrease of compliance degree, even for the highest values of E/N. In the third modification, we used a somewhat differently modified set of cross sections from the Morgan database. Modification is here made by changing the energy threshold for excitation cross sections as follows: for metastable excitation, instead of energy threshold ε=16.62 eV we put ε=18.62 eV, while for the total excitation instead of energy threshold ε=16.62 eV we put ε=19.62 eV. Cross sections for elastic momentum transfer and ionization were inserted into the code without alterations. Result of calculation of α/N with such a modified set of cross sections as entry parameter is shown by the green line in Figure 5. As we can see, this change of thresholds for excitation processes also leads to decrease in compliance degree as well as lower values of E/N, considering that only the energy thresholds of processes have been altered.

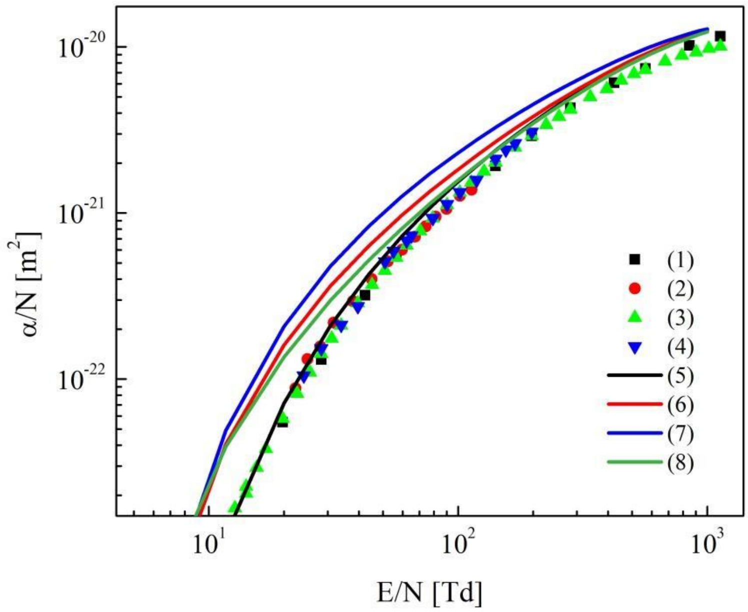

Figure 5. Reduced ionization coefficient (α/N) in function E/N for electrons in Ne gas: symbols (1), (2), (3) and (4) display measured values from Dutton database (Dutton database) while lines (5, 6, 7 and 8) present values calculated using Bolsig+ code with entry (line 5) and three modified sets of cross sections (lines 6, 7 and 8)

CONCLUSION

We presented and discussed several cross sections for e^-/Ne interaction available in the LxCat database: Biagi-v7.1, Morgan and Siglo. BOLSIG+ code was used to calculate reduced ionization coefficient (α/N) with the Morgan set of cross sections as the entry parameter and then compared it with measured values available in the Dutton database (Figure 4). The degree of compliance between calculated and measured values is satisfactory throughout the complete observed range of reduced electric field (E/N).

The swarm method was demonstrated as an example of reduced ionization coefficient (α/N) depending on reduced strength of electric field (E/N) for electrons in Ne gas. The value of this coefficient was calculated using BOLSIG+ code, where entry data was first the original set of cross sections, and then set of cross sections from the Morgan database was modified in three different ways. In the first modification, the process of metastable electron excitations was excluded (line 2 on Figure 2), while the process of total excitations was excluded in the second modification (line 3 on Figure 2). The third modification altered energy thresholds of these two excitation processes. Each modification caused a certain degree of non-compliance with measured values of transport coefficient, as shown in Figure 5, lines 6, 7 and 8. The highest degree of non-compliance of calculated values for α/N, in practically the whole range of E/N, can be noticed in the second modification, where a cross section for total excitation of energy threshold of ε=16.62 eV was excluded from the starting set.

REFERENCES

Biagi-v7.1 database. Retrieved from: www.lxcat.net (accessed April 20, 2021) .

Boltzmann, L. (1872). Weitere Studien über das Wärmegleichgewicht unter Gasmolekülen. *Sitzungsberichte Akademie der Wissenschaften*, 66, 275-370. (English translation: Boltzmann, L. (2003). Further Studies on the Thermal Equilibrium of Gas Molecules. *History of Modern Physical Sciences*, *1*, 262-349. doi.org/10.1142/9781848161337_0015

Dupljanin, S. (2016). Primjena metode elektronskih rojeva za dobijanje kompletnih presjeka i transportnih koeficijenata za azot suboksid, tetrafluoroetan i dimetil etar. (Doktorska disertacija). Fizički fakultet, Beograd.

Dutton database. Retrieved from: www.lxcat.net (accessed April 22, 2021).

Hagelaar, G. J. M. & Pitchford, L. C. (2005). Solving the Boltzmann equation to obtain electron transport coefficients and rate coefficients for fluid models. *Plasma Sources Science and Technology, 14*(4), 722–733. doi.org/10.1088/0963-0252/14/4/011

LXCat database, Plasma Data Exchange Project. Retrieved from: https://fr.lxcat.net (accessed April 20, 2021).

Morgan database. Retrieved from: www.lxcat.net (accessed April 20, 2021).

Raju, G. G. (2006). *Gaseous Electronics Theory and Practice*. Boca Raton, FL: Taylor & Francis Group LLC.

Siglo database. Retrieved from: www.lxcat.net (accessed April 20, 2021).

Tanişli, M., Mertadam, S., Poyraz, N., Şahin, N. & Demir, S. (2016). Inactivation of Microorganisms with Neon Plasma Jet at Atmospheric Pressure. *Journal of Pure and Applied Microbiology*, *10*(3), 1897-1904.

Walschus, U., Schröder, K., Finke, B., Nebe, B., Meichsner, J., Hippler, R., ... Schlosser, M. (2011). Application of Low Temperature Plasma Processes for Biomaterials. In Rosario Pignatello (Ed), *Biomaterials Applications for Nanomedicine*, (pp.127-142). Rijeka, Croatia: InTech.

Received 08 March 2022.
Accepted 08 April 2022.