International Journal of Engineering, Mathematical and Physical Sciences
ISSN: 2517-9934
Vol:5, No:11, 2011

Electron-Impact Excitation of Kr 5s, 5p Levels

Alla A. Mityureva

Abstract**—**The available data on the cross sections of electron-impact excitation of krypton 5s and 5p configuration levels out of the ground state are represented in convenient and compact form. The results are obtained by regression through all known published data related to this process.

Keywords**—**Cross section, electron excitation, krypton, regression

I. INTRODUCTION

ELECTRON collision processes with atoms and molecules have been a topic of continuous interest for both fundamental and practical reasons. Electron-impact excitation of rare gases, in particular, such as krypton for example has received considerable interest due to the importance of these noble gases in many gaseous electronic applications. These gases are heavily used in plasma processing of flat-panel displays and semiconductor manufacturing, lighting industries, gas-discharge lamps, in gas lasers, the Earth's atmosphere and molecular biology and medicine and etc. Modeling the contributions of the various processes in active environment of these sources plays an important role in understanding the basic physical properties of the plasma and aids source design. The main difficulties in such modeling arise from the necessity of rigorous treatment of electron-impact interaction, so an accurate knowledge of the excitation cross sections is crucial for this determination.

These demands have results a lot of researchers to study the electron-impact excitation's cross sections of Kr both theoretically and experimentally by a number of workers. The main emphasis has been on the determination of the total cross sections in the excitation function for incident electron energies over a wide range of its variation, but each investigator has used however only part of such region. As a rule the different workers compared own results with the work of other investigators – measured or calculated cross sections and found satisfactory consent in them, but sometimes it's obtained results that differed from the other experimental or theoretical work in both shape and magnitude, particularly, cross sections! Does this mean that this measured or a calculated cross section is not right? No. We must say that in discussed, examined cases an experimental and calculating investigations are rigorous scientific methods, and the obtained results are very good. Does this mean that we wouldn't use such results? No. In such situation therefore it is not necessary to perform a series of experiments and calculations that, one would think, will resolve these uncertainties, because they are natural uncertainties. Note that using all data published in refereed scientific journals could help to make rise of accuracy of joint result and what is the most important to make rise of reliability of joint result!

In our previous papers [1]-[5] we presented new approach to represent joint result for electron-impact excitation cross sections for a number of levels of H, He and Ar atoms. The present paper extends these results and demonstrates and analyses new combined results of electron-impact excitation's cross sections for the four 5s and ten 5p levels (Pashen's notation) of Kr atom.

II. BASIC RELATIONS

The electron-impact excitation of atoms is a fundamental collision process that occurs in a wide variety of natural and artificial active medium that is why an accurate and essentially reliable excitation cross section data are required. The cross sections of electronic rare gas atoms excitation have been measured and calculated many times but only a few of these determinations are absolute and the most of them are differ one from the other. Moreover, these data are too scattered in various literature sources. If that is so, the abundant [6]-[22] disconnected pieces of information on the constants of electronic excitation processes in Kr atoms are hindered their utilization. A user can often disregard the totality of the literature data and either relies on it's own fairly crude estimates or turns to some single source, not always the best one. As a result there is the problem of preference and choosing of available cross sections values among set of different experimental and theoretical data. What are to be done in such situation? It follows that it ought to be found some other approach for representing literature data, an approach that would represent the experience accumulated on the problem in a compact form. One of such approaches to analyzing, statistically processing, and conveniently representing both our own and literature data on the cross sections and rate constants of electronic excitation of all studied levels and spectral transitions of the atom under study was suggested by us. The method has been based on regression analysis through all known published data using parametric approximation of cross section energy dependence. We have used the approach that was introduced and developed in our previous works [1]-[5], in order to take into account all available data and obtained the summary values.

The method is based on regression through all known published data (including our own ones [6]) using parametric

A. A. Mityureva is with Faculty of Physics, Saint Petersburg State University 198504, St. Petersburg, Russia (e-mail: mitalal@mail.ru)

approximation of cross section energy dependence. We used approximation with four parameters

$$Q(E) = p_0\left(\frac{u}{u+1}\right)^{p_1}(u+p_2)^{-p_3}, \qquad u = \frac{\Delta E}{E} - 1,$$

where E is electron beam energy, ΔE is excitation threshold and p_0, p_1, p_2, p_3 are regression parameters.

The available data on the cross sections of electron-impact excitation of krypton 5s and 5p configuration levels out of the ground state:

$$\mathrm{Kr}\,(4p^6\ {}^1S_0) + e \;\rightarrow\; \mathrm{Kr}\,(4p^5 5s) + e\,,$$

$$\mathrm{Kr}\,(4p^6\ {}^1S_0) + e \;\rightarrow\; \mathrm{Kr}\,(4p^5 5p) + e$$

are presented on base of this approach.

The summery cross sections for all investigated levels are determined separately for the data including cascade population of levels from upper levels and without it – effective and direct cross sections correspondingly.

We have to observe that there are regrettable discrepancies in terminology related to the cascade population. Sometimes someone call (rather misleadingly) the experimental so-called optical values q_{ki} as the “apparent cross sections”, although these quantities represent a quite certain atomic constant, that is, the cross section for the excitation of spectral lines appearing both due to the direct electron excitation of the k_{th} level from the o_{th} state (with the cross section Q_{ok}) and due to the spontaneous cascade transitions to this level from the upper l_{th} level (with the cross section q_{lk}); the latter levels are also populated both by direct electron impact and by cascade mechanism. The optical cross sections are related to the cross section Q_{ok} for the direct electron excitation (the last value is used in the theory, which has to be compared to experiment) by the well-known expression

$$Q_{ok} = \sum_{i<k} q_{ki} - \sum_{k<l} q_{lk}\,,$$

where the summation is performed over indexes i (running from 1 to k–1) and l (from k+1 to infinity). The first term in this difference is the sum of the optical cross sections for all spectral lines emitted with the transitions from the k_{th} level to underlying levels; the second term is the sum of the optical cross sections for all cascade transitions to the k_{th} level. The first sum is called the effective cross sections, that is

$$Q_{ok} = Q_{ok}^{eff} - \sum_{k<l} q_{lk}\,,$$

$$Q_{ok}^{eff} = Q_{ok} + \sum_{k<l} q_{lk}$$

These terms: optical cross section, direct cross section and effective cross section were accepted in scientific literature on atomic and molecular physics and We believe that they more adequately reflect the essence of the phenomenon and should be preferred.

III. RESULTS

The results are obtained separately for the data including cascade population of levels from upper levels and without it – effective and direct cross sections correspondingly. The obtained data contains the regression parameters and relative sample variance D of regression for each processed transition: Tables I, III – direct cross sections and Tables II, IV – effective ones. Levels are given in Pashen’s notation.

TABLE I
DIRECT PROCESS

up level	D	$p_{0,}$ 10^{-16} cm^2	p_1	p_2	p_3
1s$_2$	0.6	1.0	2.3	0.13	0.81
1s$_3$	0.4	1.2	2.15	1.15	3.95
1s$_4$	0.5	1.4	1.62	0.16	0.73
1s$_5$	0.4	3.8	4.8	0.12	3.85

TABLE II
EFFECTIVE PROCESS

up level	D	p_0 10^{-16} cm^2	p_1	p_2	p_3
1s$_2$	0.17	1.6	2.89	0.15	0.77
1s$_3$	0.10	1.6	3.70	0.09	2.18
1s$_4$	0.14	3.1	3.04	0.15	0.77
1s$_5$	0.05	6.0	3.66	0.14	1.87

TABLE III
DIRECT PROCESS

up level	D	p_0 10^{-16} cm^2	p_1	p_2	p_3
2p$_2$	0.62	0.25	1.9	0.16	1.65
2p$_3$	0.87	0.23	3.9	0.09	4.05
2p$_4$	0.92	0.35	3.6	0.25	4.05
2p$_6$	0.57	0.22	2.1	0.15	1.95
2p$_7$	0.76	0.99	3.7	0.30	4.40
2p$_8$	0.63	0.37	2.2	0.11	1.65
2p$_9$	0.46	1.2	3.9	0.22	4.0
2p$_{10}$	0.63	1.1	3.9	0.25	3.85

TABLE IV
EFFECTIVE PROCESS

up level	D	p_0 10^{-16} cm^2	p_1	p_2	p_3
2p$_1$	0.31	0.21	2.49	0.10	0.93
2p$_2$	0.46	0.59	2.74	0.12	1.10
2p$_3$	0.47	0.21	2.53	0.12	1.20
2p$_4$	0.48	0.25	2.57	0.14	1.13
2p$_5$	0.31	0.45	2.68	0.11	0.93
2p$_6$	0.44	0.67	2.75	0.12	1.06
2p$_7$	0.58	0.74	2.87	0.13	1.14
2p$_8$	0.42	1.09	2.78	0.13	0.88
2p$_9$	0.54	0.48	2.67	0.13	1.09
2p$_{10}$	0.41	0.42	2.61	0.13	0.95

Let us note, that data spread of results of various authors for the direct cross section electronic excitation of 2p$_1$ and 2p$_5$ levels appeared to be very large and reliable cross sections could not be extracted at present.

Fig. 1-5 shows some of the results graphically. It is seen the spread of literature data and the regression curves. Vertical axis corresponds to denary logarithm of cross section Q in cm^2 and horizontal one to the electron beam energy E in eV.

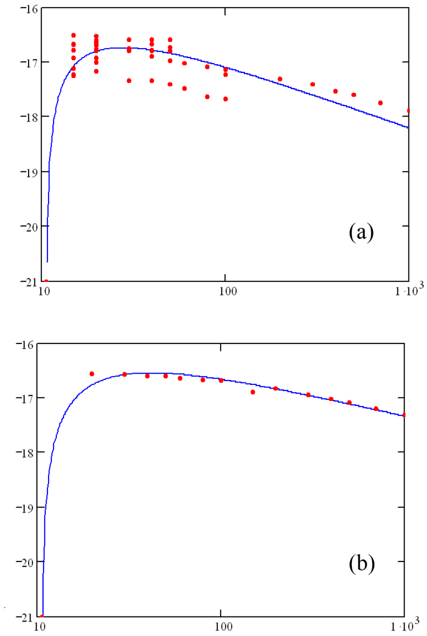

Fig. 1 Direct (a) and effective (b) excitation cross sections of $1s_2$ level

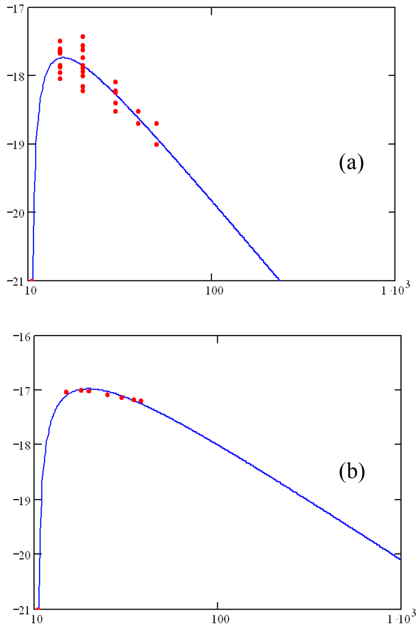

Fig. 2 Direct (a) and effective (b) excitation cross sections of $1s_3$ level

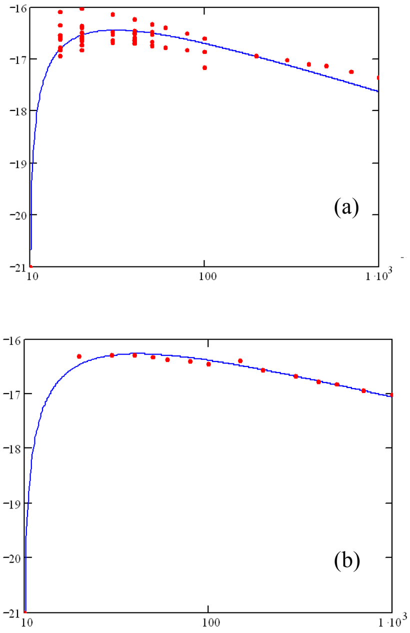

Fig. 3 Direct (a) and effective (b) excitation cross sections of $1s_4$ level

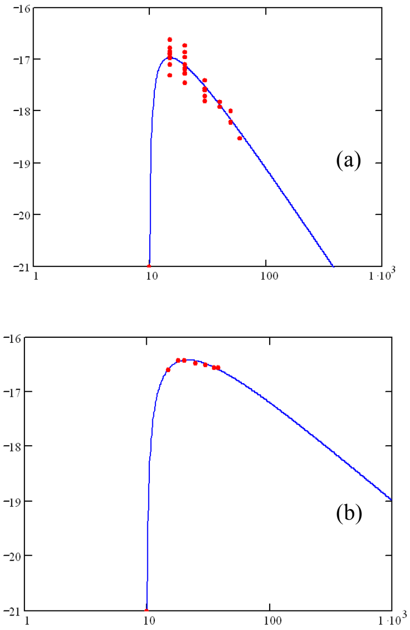

Fig. 4 Direct (a) and effective (b) excitation cross sections of $1s_5$ level

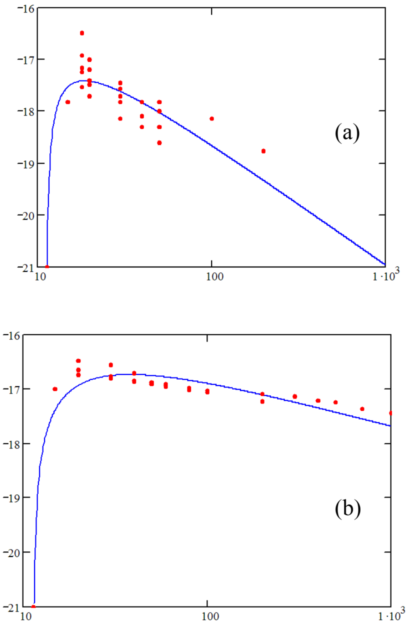

Fig. 5 Direct (a) and effective (b) excitation cross sections of $1p_{10}$ level

It is seen that the shape of the direct excitation functions of metastable levels $1s_3$, $1s_5$ are more sharp then for the resonance levels $1s_2$, $1s_4$. This difference almost vanishes for the effective excitation functions almost vanishes.

IV. CONCLUSION

The obtained data is a compact and convenient representation of totality of all available data and can be valuable for various applications. It is more reliable than data of concrete sources taken separately. It permits to quantitatively observe differences between direct and effective cross sections. For example, the difference in direct cross sections of metastable s_3, s_5 and resonance s_2, s_4 levels are very large, as for the effective cross sections – they are nearly equal. For p levels effective cross sections becomes almost equal too.

REFERENCES

[1] A. A. Mityureva, V. V. Smirnov. Electron Excitation Cross-Section Energy Behaviour Approximation for Helium Atom. Opt & Spectr. 1993, v. 74, n. 1, p. 6-11

[2] A. A. Mityureva, V. V. Smirnov. Approximation of energy dependences of the cross sections for electron excitation of atomic levels of helium from metastable states. Optics & Spectroscopy. 1999, v. 86, n. 6, p. 833-837

[3] A. A. Mityureva, V. V. Smirnov, G. A. Ponomarenko. Approximation of the Electron Excitation Cross Sections for Triplet States Excited from the 2^3S_1 Metastable State in Helium. Optics & Spectroscopy, 2002, v. 92, n. 3, p. 325-331

[4] A. A. Mityureva, V. V. Smirnov. Electronic Excitation of Ar Atoms to Metastable States and from Metastable to Higher States. Optics & Spectroscopy, 2004, v. 97, n. 4, p. 508-521

[5] A. A. Mityureva, V. V. Smirnov. Integral Electronic Excitation Cross Sections of Hydrogen Atom Levels. Optics & Spectroscopy, 2006, v. 101, n. 3, p. 338-343

[6] A. A. Mityureva, V. V. Smirnov. Excitation of heavy rare gases to metastable states by electron impact. J. Phys. B: Atomic & Mol. Phys., 1994, v. 27, n. 9, p.1869-1880

[7] Dasgupta A.,Bartschat K., Vaid D., Grum-Grzhimailo A.N., Madison D.H., Blaha M. & Giuliani J.L. // Phys. Rev.A.2001> V.64, 052710.

[8] Kaur S., Srivastavay R., McEachran R.P. & Stauffer A.D. // J. Phys.B. 1998. V.31, p. 4833

[9] P. V. Feltsan. Ukr. Phys. J., 1967, v. 12, p. 1425 (Russian)

[10] [S. Tsurubuchi, H. Kobayashi and M. Hyodo // J. Phys. B. 2003. V. 36, 2629

[11] J. Ethan Chilton, M. O. Stewart, Jr. and Chun C. Lin // Phys. Rev.A. 2000. V. 62, 032714.

[12] I. P. Bogdanova, S. V. Yurgenson. Optics & Spectroscopy. 1987, v. 62, p. 713

[13] Xuezhe Guo, D.F.Mathews, G.Mikaelian, M.A.Khakoo, A.Crowe, I.Kanik, S.Trajmar, V.Zeman, K.Bartschat and C.J.Fontes // J. Phys. B. 2000. V.33, 1895

[14] S. Trajmar, S.κ. Srivastava, H. Tanaka and H. Nishimura. // Phys. Rev. A.1981. V. 23, p. 2167.

[15] V. Kaufman // J. Res. Nat.Inst. Stand. Tech. 1993. V.98, 717

[16] N.J. Mason and W.R. Newell // J. Phys. B. 1987. V.20, 1357.

[17] T. Takayanagy, G.P.Li, K. Wakiya, H. Suzuki, T. Ajiro, T. Inaba, S.S. Kano and H. Takuma // Phys. Rev. A.1990. V. 41 p. 5948.

[18] Xuezhe GuO, D.F.Mathews, G.Mikaelian, M.A.Khakoo, A.Crowe, I.Kanik, S.Trajmar, V.Zeman, K.Bartschat and C.J.Fontes // J. Phys. B. 2000. V.33, 1921

[19] G. D. Meneses, F. J. da Paixo and N. T. Padial // Phys. Rev. A. 1985. V. 32, p.156.

[20] J. M. Phillips // J. Phys. B. 1982. V. 15, 4259

[21] N. Swanson, J. W. Cooper and C. E. Kuyatt // Phys. Rev. A. 1973.V.8, 1825

[22] P. A. Pavlov, V. E. Yahontova. Optics & Spectroscopy. 1975, v. 39, p. 229