TOTAL ELECTRON EXCITATION CROSS SECTIONS FOR LOW-ENERGY AUTOIONIZING STATES IN LITHIUM

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The total electron impact excitation cross-sections have been obtained for the first time for the $(1s2s^2)^2S$, $(1s2s2p)^4P_{1/2,3/2}$, $1s(2s2p^3P)^2P$ and $1s(2s2p^1P)^2P$ autoionizing states in lithium atoms by normalizing the experimental relative cross-sections to the PWBA calculations at 600 eV. The maximum values of the cross-sections lie in the range of $0.3 \div 1.0 \times 10^{-18}$ cm^2. The contribution of negative-ion resonances and resonance cascades to the excitation of autoionizing states has been analyzed.

The lowest $(1s2s^2)^2S$, $(1s2s2p)^4P_{1/2,3/2}$, $1s(2s2p^3P)^2P$ and $1s(2s2p^1P)^2P$ -autoionizing states of lithium due to their large energy separation ($\Delta E \geq 1$ eV) are very convenient for the experimental investigation by the electron spectroscopy method. The systematic investigation of electron impact excitation of these states gives a unique possibility to study the dynamics of electron-atom interaction even staying in the frame of the L-S coupling scheme. Being of different type relatively to their excitation and decay processes, these states are the good probes also for revealing the influence of electron correlation effects in the different electron subshells. Moreover, for lithium atoms the radiative transitions between the autoionizing states both in the quartet and doublet systems are very efficient [1,2]. The $(1s2s2p)^4P_{1/2,3/2}$, and $1s(2s2p^3P)^2P$ states are radiatively connected with the most of high-lying autoionizing states and this allows one to study also the character of such cascade transitions and evaluate their common contribution to the electron impact excitation process.

Many experimental and theoretical works were published at present time on the autoionization in lithium atoms (see e.g. [1,3] and references therein). However, the main attention of the authors was paid to the spectroscopic parameters of autoionizing states, i.e. excitation energies, decay channels, lifetimes etc. [2-4]. As to the excitation cross-sections, the only experimental work of Feldman and Novick [5] is known on determination of the electron impact excitation cross-section for the $(1s2s2p)^4P_{5/2}$ metastable autoionizing state. The theoretical calculations of the excitation cross-section are only known for the lowest lithium $(1s2s^2)^2S$ state. In [6,7] by using the plane-wave Born approximation (PWBA) the maximum value of the total cross-section of $2.2 \cdot 10^{-19}$ cm^2 has been obtained for this state. In more systematic calculations of Pangantivar and Srivastava [8] the distortion-wave approximation (DWA) has been used with including the polarization and exchange effects. In the last case an evident resonant character of the electron excitation for the $(1s2s^2)^2S$ level has been revealed with the maximum value of the total cross-section of $7.4 \cdot 10^{-19}$ cm^2 at 59 eV.

Recently we have reported the data on the ejected-electron excitation functions for the $(1s2s^2)^2S$, $(1s2s2p)^4P_{1/2,3/2}$, $1s(2s2p^3P)^2P$ and $1s(2s2p^1P)^2P$ -autoionizing states in lithium atoms [9].The measurements were performed on the apparatus consisted of a 127° electrostatic ejected-electron analyzer, an electron gun and a resistively heated atomic beam source [10]. The energy spread of incident electrons was ≈ 0.4 eV (FWHM) as it was determined from the elastic scattering peak. The excitation functions have been obtained in the form of impact energy dependences of the normalized ejected-electron intensities measured at an observation angle $\theta = 54.7°$. Note that the ejected-electron excitation functions obtained in these measurements reflect the incident energy dependences of the total electron excitation cross-section for autoionizing levels.

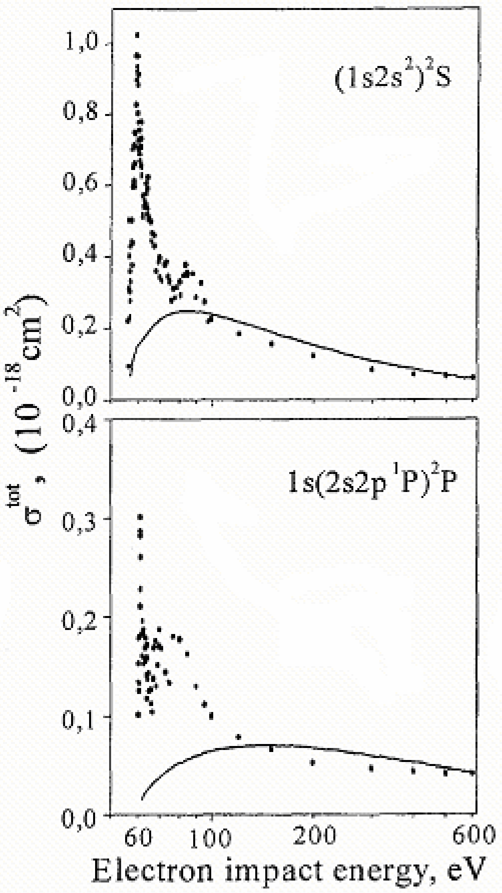

Fig. 1. Total electron impact excitation cross-sections for the $(1s2s^2)^2S$ and $1s(2s2p^1P)^2P$ autoionizing levels in lithium: (•) - experiment [9]; (—) - present PWBA calculations.

With the aim of normalization of the experimental relative cross-sections obtained in [9] here we have performed the PWBA calculations of the $1s^22s \rightarrow 1s2snl$ excitation process for the $(1s2s^2)^2S$ and $1s(2s2p^1P)^2P$ - autoionizing states in lithium. The procedure for generating the target wavefunctions has been described earlier [11]. Briefly, we used the Froese Fisher multiconfiguration Hartree-Fock (MCHF) atomic structure package [12] with the special attention paid to the large relaxation both of the 1s and *nl* orbitals at the 1s excitation and to the correlation corrections arising from the strong interaction between the 1s electrons. The spectroscopic 1s, 2s and 2p orbitals were obtained from the Hartree-Fock calculation of the $(1s2s2p)^4P$ state. The 3s, 3p and 3d correlation orbitals were generated from the optimization of the $(1s2s2p)^4P$ state in the MCHF calculations in the active space manner. The final multiconfiguration expansion for all terms of interest have been obtained by the configuration-interaction method on the basis of all possible configurations constructed from the above spectroscopic and correlation orbitals.

Figure 1 shows a comparison of the experimental [9] and present theoretical results at the incident electron energies up to 600 eV for the $(1s2s^2)^2S$ - and $1s(2s2p^1P)^2P$ - autoionizing states. For the normalization of theoretical data we have choosen the $(1s2s^2)^2S$ state due to the abscence for it of the cascade transitions [1]. The normalization has been done at an incident electron energy of 600 eV that is satisfies the known condition of validity of the Born approximation $E_o \geq 10E_{exc}$ where E_{exc} is the excitation energy of an autoionizing level [13]. As can be seen, above 200 eV there is a good agreement between both data. The results of normalization are shown in Fig. 2 for all autoionizing states studied. The maximum values of the cross-sections σ^{tot}_{max} are given in Table 1 together with other data known for these levels.

Table 1. Total excitation cross-sections σ^{tot}_{max} for the lowest autoionizing states in lithium

State	σ^{tot}_{max} $(10^{-18}\ cm^2)$				
	Experiment	Theory			
	Present data	Present data, PWBA	[6], PWBA	[7], PWBA	[8], DWE
$(1s2s^2)^2S$	1.0	0.25	0.22	0.22	0.74
$(1s2s2p)^4P_{1/2,3/2}$	0.7	–	–	–	–
$1s(2s2p^3P)^2P$	1.0	–	–	–	–
$1s(2s2p^1P)^2P$	0.3	0.07	–	–	–

Comparing these data one can see that for the $(1s2s^2)^2S$ state all PWBA calculations give the values of the $\sigma^{tot}{}_{max}$, which are smaller than the experimental data approximately by the factor of four. The result of the DWE approach [8], which takes into account the exchange character of electron excitation for the $(1s2s^2)^2S$ state, is much closer to the experiment (see Fig. 3). The higher experimental value of the cross section in this case is caused by the presence of the strong negative-ion resonance just on the top of the main maximum at 59.5 eV [9].

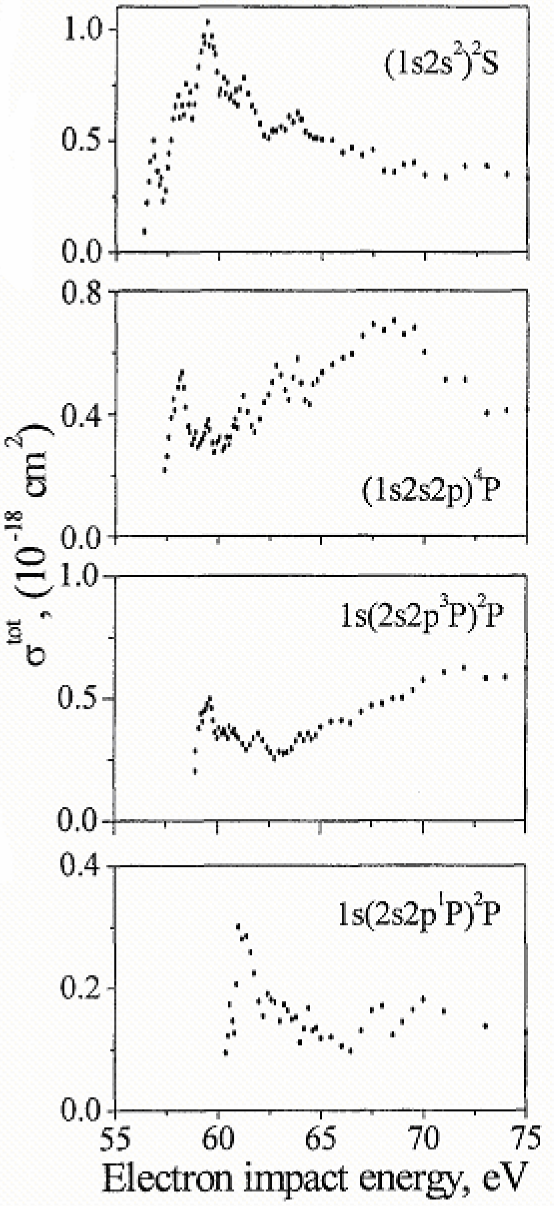

Fig. 2. Total electron impact excitation cross-sections for the low-energy autoionizing states in lithium.

Another result of the present work is the evaluation of the excitation cross-sections for the negative-ion resonances revealed above the excitation thresholds of all levels considered (Fig. 2). As one can see, for the $(1s2s^2)^2S$ and $(1s2s2p)^4P$ states these cross-sections reach the value of 70% of the $\sigma^{tot}{}_{max}$ showing the dominant resonance character of the near-threshold electron excitation of these levels. The resonance processes dominate also at the excitation thresholds of the 1s2s2p doublet levels.

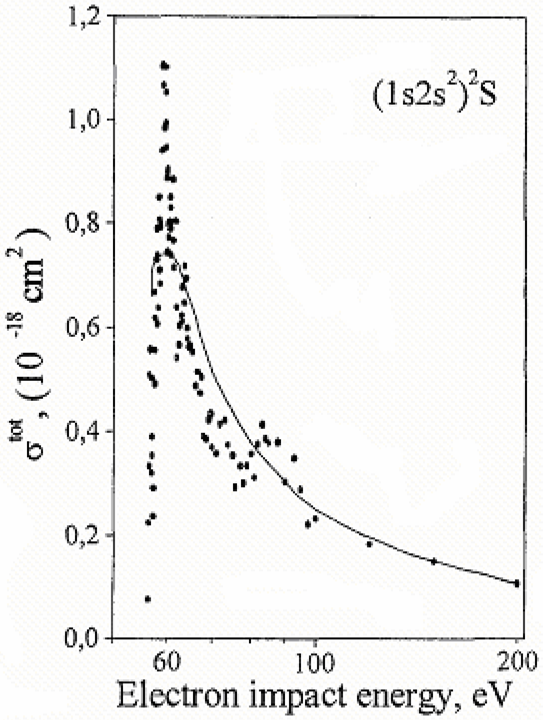

Fig. 3. Total excitation cross-section for the $(1s2s^2)^2S$ autoionizing state: (—) - DWE calculations [8]; (•) – experiment [9] normalized to theory [8] at 200 eV.

In accordance with the spectroscopic data [1,2] the $(1s2s2p)^4P_{1/2,3/2}$ level is the final state for the most of radiative transitions known in the quartet level system of lithium [1]. The contribution from the radiative cascades to the excitation cross-section of this level has been found to be the largest and equal 30%. On the other hand, such contribution for the lowest doublet $1s(2s2p^3P)^2P$ has been found to be 3% only.

In conclusion, the total electron impact excitation cross-sections for the lowest $(1s2s^2)^2S$, $(1s2s2p)^4P_{1/2,3/2}$, $1s(2s2p^3P)^2P$ and

$1s(2s2p^1P)^2P$ -autoionizing states in lithium atoms have been determined by normalizing the relative experimental excitation functions to the PWBA calculations at 600 eV impact energy. The data give the quantitative information on the role of the resonance and cascade processes in electron excitation of low-lying autoionizing states in lithium atoms. We hope that the results obtained could be a good base for the further theoretical calculations of the inner-shell excitation in lithium atoms.

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References

1. S.Mannervik, H.Cederquist, *Physica Scripta* **27,** 175 (1983).
2. U.I.Safronova, V.S.Senashenko, *Opt. Spectrosc.* **42,** 462 (1977).
3. H.Cederquist, S.Mannervik, *Phys. Rev. A* **31,** 171 (1985).
4. A.V.Kupliauskiene. Z.J.Kupliauskis, In: *Autoionization phenomena in atoms and ions* (Moscow University Press, Moscow, 1983) p. 5–33 [in Russian].
5. P.Feldman, R.Novick, *Phys. Rev.* **160,** 143 (1967).
6. R.Srivastava, C.S.Singh, D.K.Rai, *J. Phys. B* **15,** 1899 (1982).
7. S.N.Tiwary, J.Macek, D.H.Madison, *Phys. Rev. A* **32,** 2541 (1985).
8. A.W.Pangantiwar, R.Srivastava, *J.Phys. B* **20,** 5881 (1987).
9. A.A.Borovik, V.N.Krasilinec, *J. Phys. B* **32,** 1941 (1999).
10. O.O.Borovik, *Ukr. J. Phys.* **45,** 1270 (2000).
11. O.Zatsarinny, *J. Phys. B* **32,** L565 (1999).
12. C.Froese Fischer, *Comput. Phys. Commun.* **64,** 1991 (1991).
13. H.S.W.Massey, E.H.S.Burhop, *Electronic and Ionic Impact Phenomena* (Oxford, 1952)

ПОВНІ ПОПЕРЕЧНІ ПЕРЕРІЗИ ЕЛЕКТРОННОГО ЗБУДЖЕННЯ НИЗЬКОЕНЕРГЕТИЧНИХ АВТОІОНІЗАЦІЙНИХ СТАНІВ ЛІТІЮ

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Вперше одержані повні поперечні перерізи електронного збудження $(1s2s^2)^2S$, $(1s2s2p)^4P_{1/2,3/2,}$ $1s(2s2p^3P)^2P$ та $1s(2s2p^1P)^2P$ автоіонізаційних станів атома літію шляхом нормування експериментальних відносних поперечних перерізів на ПХНБ розрахунки при енергії 600 еВ. Максимальні значення поперечних перерізів лежать в діапазоні $0.3 \div 1.0 \times 10^{-18}$ см^2. Проаналізовано внесок резонансів негативного іона і каскадних резонансів при збудженні автоіонізаційних станів.