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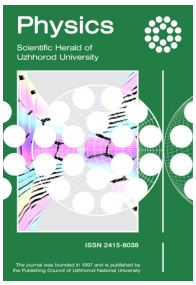

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Theoretical Calculations of Electron Excitation of the Lowest Autoionization States of the Rb Atom

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Abstract

Purpose. The value of the autoionization cross section and its energy dependence are determined to a great extent by excitation and subsequent electron decay of the lowest energy states. Recently, experimental data on the excitation cross sections of the rubidium atom lowest doublet $(4p^5 5s^2)^2P_{3/2,1/2}$ and quartet $(4p^5 4d5s)^4P_{1/2,3/2,5/2}$ autoionizing states were obtained which promoted their theoretical investigations.

Methods. Theoretical calculations were performed using the Flexible Atomic Code universal program package which takes account of the relativistic nature of the complex atoms excitation by the use of the Dirac-Coulomb Hamiltonian. The radial orbitals for basic relativistic wavefunctions were obtained by solving the Dirac-Fock-Slater equation.

Results. Comparison of the experimental excitation cross sections for the doublet $(4p^5 5s^2)^2P_{3/2,1/2}$ and quartet $(4p^5 4d5s)^4P_{1/2,3/2,5/2}$ autoionizing states with available theoretical data and our relativistic calculations is presented. The results of the study of the parameter R_0 for the intensity ratio for the $^2P_{3/2}$ and $^2P_{1/2}$ states of the $4p^5 5s^2$ configuration are presented. Our calculations in the distorted waves approximation is shown to well describe the experimental data in the energy region above 70 eV. At low collision energies our calculations qualitatively predict the presence of the threshold resonant excitation; however in the energy region 20-50 eV only the R-matrix method qualitatively describes the complex nature of excitation and decay of the lowest quartet autoionizing states of the rubidium atom.

Conclusions. Electron excitation of the doublet $(4p^5 5s^2)^2P_{3/2,1/2}$ and quartet $(4p^5 4d5s)^4P_{1/2,3/2,5/2}$ autoionizing states of the rubidium atom in the collision energy range from the excitation thresholds up to 700 eV was studied in the terms of the distorted waves relativistic approximation. A comprehensive analysis of the obtained results using the available experimental and theoretical data showed that the relativistic distorted waves approximation taking into account the configurational mixing is a suitable tool for describing the autoionizing states of the rubidium atom in a wide range of collision energies and allowed one to obtain the absolute values of the experimental excitation cross sections of the $(4p^5 5s^2)^2P_{3/2,1/2}$ and $(4p^5 4d5s)^4_{P1/2,3/2,5/2}$ states.

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Keywords: atom, electron impact excitation, autoionizing states, excitation cross section

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Introduction

The charge composition and energy balance of various plasma media are mainly determined by two processes – direct ionization and autoionization. As has been shown in studies of these processes in heavy atoms of potassium, rubidium and caesium [1], the contribution of autoionization to the total electron shock ionization cross-section is more than 30%. Studies of these atoms have also shown that the size of the autoionization cross-section and the form of its energy dependence at low and high collision energy values are largely determined by the excitation and subsequent electronic decay of the lowest-energy states $np^5(n+1)s^2\ ^2P_{3/2,1/2}$ and $np^5nd(n+1)s\ ^4P_{1/2,3/2,5/2}$ (n=3, 4, 5 for K, Rb, Cs, respectively) [2-4].

It is known that the most complete information about the set of processes involved in the formation of a certain excited atomic state, namely the type of electron transition, cascade population, and the formation of negative ion resonances, is provided by the energy dependence of its excitation cross-section. Recently, by the method of electron spectroscopy using the technique of electron-atom beams, it was possible to experimentally obtain cross sections of the excitation of the lowest autoionization states (AIS) for the Rb atom [5-7]. Due to the significant spin-orbit splitting of levels in the Rb atom, apart from the doublet states $(4p^55s^2)^2P_{3/2,1/2}$ [5], in the study [6] the electronic excitation of each component with J=1/2, 3/2, 5/2 of quartet state $(4p^54d5s)^4$RJ was also studied. Detailed analysis of the near-threshold resonant structure of AIC data performed by the authors in the study [8]. In it, on the basis of theoretical calculations by the method of R-matrix with B-splines show that the resonant structure at the excitation cross-sections for $(4p^55s^2)^2P_{3/2,1/2}$ AIC is the result of a superposition of several states of the negative rubidium ion, and it is also established that almost all resonances are Feshbach-type resonances. As for the quartet AIC, the authors of the study [8] presented the excitation cross-sections of these AIC in the collision energy range up to 50 eV, but they were unable to identify the states of the negative rubidium ion due to the complexity of the excitation and decay mechanism of these AIC.

As for collision energies above 50 eV, only one theoretical work has been known so far [9], where the excitation cross-sections are presented and the role of $np^5(n+1)s^2\ ^2P_{3/2,1/2}$ AIC in the process of ionization of neutral alkaline atoms by electron shock. In this research, relativistic calculations of effective excitation cross-sections in the Born approximation and distorted waves (PCX) are performed, multiplet splitting analysis is performed, and the ratio of the cross-sections of the lowest doublet AIC of alkaline Na, K, Rb, and Cs atoms at different energies of the incident electron from the excitation thresholds to 1.5 keV is established, but without comparison with experimental data for Rb and Cs atoms. For quartets $(4p^54d5s)^4$RJ AIS theoretical data on excitation cross-sections for collision energies above 50 EV were not available.

In this study, we present the results of a theoretical study of the electron excitation of the lowest doublet and quartet autoionization states of a rubidium atom in a wide range of collision energies from excitation thresholds to 700 eV by the method of relativistic distorted waves, taking into account configuration mixing (the PCX-BK approximation) and without it (the PCX approximation) in comparison with the available theoretical and experimental data.

Research Methodology

Theoretical calculations were performed using the universal Flexible Atomic Code software package [10], which takes into account the relativistic nature of the excitation of complex atoms by using the Dirac-Coulomb Hamiltonian. This software package has proven itself well in the theoretical classification of AIC of the rubidium atom in the research [11], as well as in the study

of the excitation cross-section $4p^6$ shells of the Rb atom [12; 13].

It should be noted that the accuracy of the theoretical results obtained significantly depends on how the single-electron functions of the target are calculated and what configurations are mixed with each other. Clearly, there is no universal recipe for how to improve the results of calculations, it all depends on successful and complete consideration of configuration mixing. At the same time, the number of configurations cannot be excessively large, since it is impossible to take into account the interaction of an incoming electron with all possible configurations. Mixing of configurations is usually the largest when the energies of different configurations are close to each other, it can disrupt serial patterns and even change the nature of the multiplet separation of levels. Therefore, taking into account configuration mixing in such cases often leads to significant changes in the probability of decay of individual AIC, especially for weak transitions.

Radial orbitals for constructing basic relativistic wave functions were obtained by solving the Dirac-Fock-Slater equation. The set of configurations was somewhat reduced in comparison with [11], as our research showed that the best description of experimental excitation cross-sections is given by the inclusion of correlation corrections in the calculations of our selected configurations, although excitation energies have greater differences with experimental values. To optimize the local central potential, which should reflect the polarization of the frame containing the exchange member, the following one-electron configurations were used $4p^6nl$ (n=5, 6, 7, l=0, 1, 2, 3). To account for correlation effects (BK) the following configurations were used $4p^6nl$ (n=5, 6, 7, l=0, 1, 2, 3), $4p^5nln'l'$ (nl=5s, 6s, 5p, 4d, 5d, $n'l'$=5s, 6s, 5p, 6p, 4d, 5D, 4f, 5f, 5G) for the main $4p^65s$ state of the Rb Atom and for $4p^6$, $4p^5nl$ (nl=5s, 6s), $4p^4nln'l'$ (nl=5s, 5p, $n'l'$=5s, 5p, 4D, 5D) the final state of Rb+. Calculations were performed in *jj* connections.

Results and Discussion

In Figure 1 presented a comparison of experimental excitation cross-sections [5] of doublet $(4p^55s2)^2P_{3/2,1/2}$ AIC with our theoretical calculations and data [9]. The experimental data were normalized to our RCX calculations at a collision energy of 650 eV. In the region of energies above 100 eV, our theoretical excitation cross-sections of PCX and PCX-BK $(4p^55s^2)^2P_{1/2,3/2}$ states within the experimental error satisfactorily describe the experimental data. Born and PCX excitation cross-sections [9] in this energy range underestimate the absolute values of the cross-sections. However, it should be noted that both our data and the data [9] correspond to the rule of the ratio of cross-section values $^2P_{3/2}$:$^2P_{1/2}$≈2:1 [14]. Why is it correct to normalize for our data for comparison, and not for data [9]? According to the data [8], and the R-matrix method is the most accurate method for calculating cross-sections in the near-threshold energy range, the excitation cross-sections should have even higher absolute values of effective cross-sections, i.e. our data are closer to them. In this figure, comparison with them is not given, since the excitation cross-sections $(4p^55s^2)^2P_{1/2,3/2}$ states in [8] are represented in a very narrow range of 15-20 eV.

A significant difference between experiment and theory exists for small and medium values of collision energy. Worth noting that the description of processes in the range of energies of 20-90 EV is an issue for all existing theoretical approximations, since it requires simultaneous consideration of a large number of high-energy configurations as $4p^6$ shell and excitation from the deeper shells of the rubidium atom. It is also necessary to take into account the contribution of possible cascade and radiation transitions, which is a very complex theoretical problem. Indeed, as the analysis of the experimental cross-section of the excitation state $(4p^55s^2)^2P_{1/2}$ shows, at collision energies of 18-30 eV, oscillatory behaviour and an increase in the cross-section value of up to 20% are observed. As follows from [15] in the wavelength range from 624 to 577 Å (19.8-21.5 eV), the photoabsorption

spectrum of the $4p^6$ shell contains a total of 46 lines, of which only 8 have an extended autoionization profile. This means that most AIC located above 19 eV decay mainly due to radiation transitions to low-energy AIC, in particular $(4p^55s^2)^2P_{1/2}$. Regarding the cross-section of the excitation state $(4p^55s^2)^2P_{3/2}$, then in the energy range of 20-30 EV, the noticeable effect of cascading population processes from high-energy levels is not observed. The PCX-BR approximation best describes the excitation process in this region. The figure shows that in the near-threshold region of collision energies, the experimental data of both levels have a distinct resonant character. The size of the cross-sections of the latter exceeds the efficiency of the direct process by almost one and a half times. Detailed analysis of this section in [8] showed that all resonances here are Feshbach-type resonances with a common 4p configuration $^5 6s^5p^2$ in the case of $(4p^55s^2)^2P_{3/2}$ and a common configuration $4p^55s4d6s$ for autoionization state $(4p^55s^2)^2P_{1/2}$. Theoretical approximations of PCX and Born in the near-threshold region of collision energies cannot qualitatively describe such resonant processes.

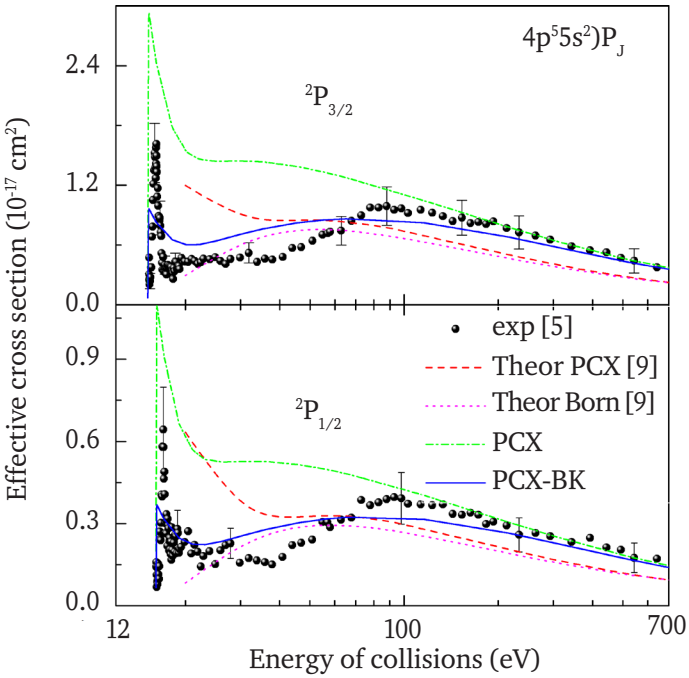

Figure 1. Effective cross-sections of doublet excitation $(4p^55s^2)^2P_{3/2,1/2}$ AIC of the rubidium atom

The cross-section of the PCX without taking into account configuration mixing significantly overestimates the efficiency of near-threshold excitation, but still assumes its presence, as well as the approximation of the PCX [9]. The calculations performed in [9] in the Born approximation do not take into account the possibility of resonant excitation, as evidenced by the behaviour of the corresponding excitation cross-section in the near-threshold region of collision energies. Since the Born approximation is a scattering in a potential field, it does not describe the details of the scattering process at low collision energies. Although the PCX-BK approximation differs from the experimental data in the near-threshold region, it also predicts a sharp increase in the efficiency of resonant excitation of AIC data. This indicates that the method takes into account to a greater extent the perturbations of the incoming and scattered waves by the field of the atomic residue and, at the excitation threshold, provides for the possibility of capturing the incoming electron in the discrete spectrum state with simultaneous excitation of the bound electron from the inner shell.

In our research, the ratio parameter

$R_0 = {}_{\sigma 3/2/\sigma 1/2}$ of line intensities $(4p^5 5s^2)^2P_{3/2}$ and $(4p^5 5s^2)^2P_{1/2}$, which according to [14] should be correlated as 2: 1 or 100% to 50% is also studied. In Figure 2 experimental data are compared with theoretical calculations in the Born approximation, PCX and relativistic approximation of distorted waves with exchange (PCXO) [9]. The general behavior of the dependence of the ratio of experimental line intensities is characterized by a sharp near-threshold resonance, an oscillatory structure up to 30 eV, and then an almost linear classical dependence up to 650 eV. This behaviour is primarily due to the dominant role of negative ion States in the near-threshold excitation of AIC $(4p^5 5s^2)^2P_{3/2,1/2}$, and the influence of cascade population at energies up to 30 eV, which has already been discussed above. Theoretical calculations of PCX and Born in the region of collision energies up to 30 eV, as already shown in the description of excitation cross-sections, differ significantly. It is difficult to talk about the quality of theoretical values of the ratio parameter R_0 in this area since the experimental data also have a large spread of values, but as can be seen, there is a perfect coincidence of our theoretical calculations of the RCX with the RCX data [9], both with and without exchange. Nevertheless it is necessary to note the remarkable coincidence of theoretical and experimental data in the region of collision energies of 35-650 eV. This means that in the case of theoretical calculations of the PCX in the strong coupling decomposition, configurations are successfully selected that take into account the correlation mixing of levels and the correctly selected model potential used to determine single-electron radial wave functions. Also, such a good agreement shows the reliability of experimental measurements.

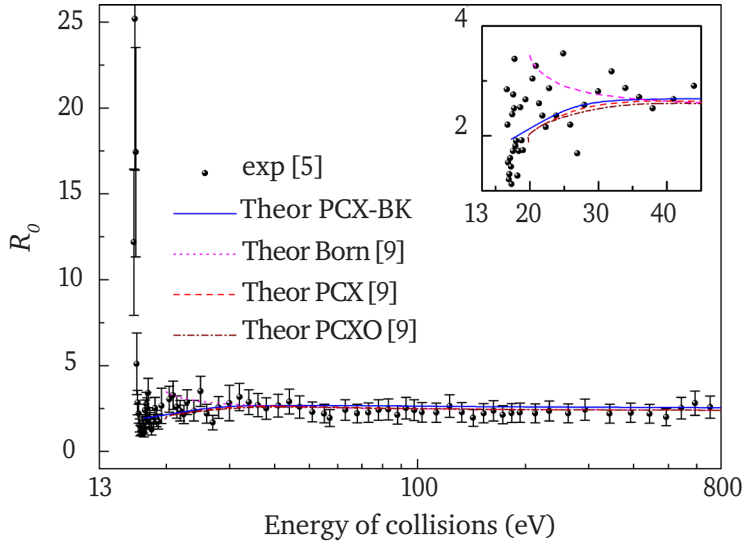

Figure 2. Intensity ratio $R_0 = \sigma_{zb}[(4p^5 5s^2)^2P_{3/2}]/\sigma_{zb}[(4p^5 5s^2)^2P_{1/2}]$ AIC of the rubidium atom

Figure 3 shows the experimental excitation cross-sections [6] of the lowest quartets $(4p^5 4d5s)^4P_{1/2,3/2,5/2}$ AIC in comparison with our theoretical calculations of PCX-BK in the range of collision energies of 16-700 eV and R-matrix with B-splines data [8] (16-50 eV).

Experimental data are normalized to PCX-BK data at a collision energy of 350 eV for states $^4P_{3/2,5/2}$ and 110 eV for $^4P_{1/2}$. It should be noted that in the case of quartet AIC, the PCX method without correlation corrections gave unsatisfactory results, which were rejected. This indicates the complexity of the process of excitation and decay of these states, as well as the fact that configuration mixing plays a more significant role here. The general view of all experimental cross-sections is broadly similar and reflects the exchange nature of excitation of these quartet levels. Although theoretical data differ significantly in general behavior, but in absolute terms correlate well with each other when describing experimental data. Both types of theoretical data do not

contradict the rule of correlation of the intensity of spectral lines within the same series $^4P_{5/2}$:$^4P_{3/2}$:$^4P_{1/2}$≈3:2:1 [14]. All functions start with intense narrow maxima (ΔE<1 eV), which are located just beyond the excitation threshold, indicating the presence of effective resonant excitation in the near-threshold energy region, as indicated by studies [8] and our theoretical calculations. In the energy range of 17-24 eV, a slight increase in the excitation efficiency is noticeable at all cross-sections, which is most clearly manifested for the level of $^4P_{1/2}$.

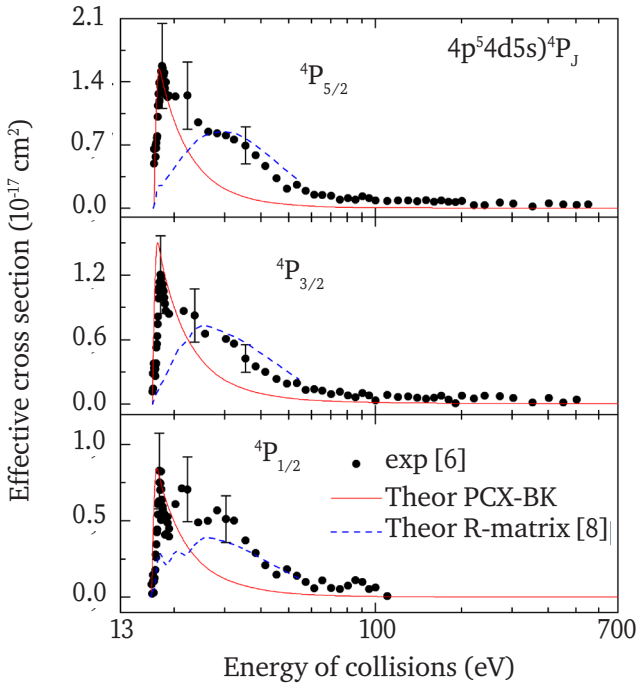

Figure 3. Effective quartet excitation cross-sections $(4p^54d5s)^4P_{1/2,3/2,5/2}$ AIC of the rubidium atom

This increase in cross-section has a cascading origin due to the radiation decay of high-energy states. If our theoretical calculations in this region significantly underestimate the values of all excitation cross-sections, then the data [8] perfectly predict an increase in the cross-section size due to the presence of additional input as a result of radiation decay from the upper 4p levels ^{5}4d5s, 4p^{5}5s5p, 4p^{5}5p^2, 4p^{5}4d5p configurations. The disadvantage of our theoretical calculations is precisely the impossibility to take into account cascade transitions, a very difficult theoretical problem indeed. In the region of collision energies above 70 eV, our theoretical PCX-BK data qualitatively describe the excitation process of quartet AIC data, which allows us to normalize experimental data in order to obtain absolute values of effective excitation cross-sections $(4p^54d5s)^4P_{1/2,3/2,5/2}$ AIC of the rubidium atom. The excitation energies and absolute values of the experimental excitation cross-sections obtained during normalization for our theoretical calculations of PCX-BK are shown in Table 1.

Table 1. Figure 1: Calculated and experimental electron excitation energies (E_{zb}, eV), excitation cross-sections (σ, 10^{-17} cm^2) in maxima σ_{max} and at collision energies of 100 and 500 eV, as well as the probability of electron decay (A, c^{-1}) AIS $4p^5nl(L_1S_1)n'l'LSJ$ the rubidium atom

$(L_1S_1)LSJ$	E_{zb}, calculation	E_{zb}, experiment [12]	σ, 10^{-17} см^2			A, c^{-1}
			σ_{max}	≈ 100 eV	≈ 500 eV	
$5s^2\ ^2P_{3/2}$	15.134	15.31	1.61	0.92	0.47	$7.65\cdot10^{12}$
$5s^2\ ^2P_{1/2}$	16.040	16.16	0.64	0.37	0.20	$1.04\cdot10^{13}$
$4d(^3P)5s\ ^4P_{1/2}$	16.665	16.69	0.08	0.06	0	$9.08\cdot10^{8}$
$4d(^3P)5s\ ^4P_{3/2}$	16.754	16.79	1.21	0.08	0.04	$6.12\cdot10^{7}$
$4d(^3P)5s\ ^4P_{5/2}$	16.907	16.97	1.57	0.08	0.03	$5.31\cdot10^{11}$

Conclusions

The study presents a comparison of experimental cross-sections of doublet excitation $(4p^55s^2)^2P_{3/2,1/2}$ and quartet $(4p^54d5s)^4P_{1/2,3/2,5/2}$ autoionization states with available theoretical data and our relativistic calculations. The results of the study of the parameter R_0 of the intensity ratio for the states $^2P_{3/2}$ and $^2P_{1/2}$ configuration $4p^55s^2$ are presented. It is shown that in the region of energies above 70 eV, our calculations in the approximation of distorted waves well describe the experimental data. At low collision energies, our calculations qualitatively predict the presence of near-threshold resonant excitation, and in the tange of average energies of 20-50 EV, only the R-matrix method qualitatively describes the complex nature of excitation and decay of the lowest quartet autoionization states of the rubidium atom. A comprehensive analysis of the obtained results with the involvement of available experimental and theoretical data showed that the approximation of relativistic distorted waves, taking into account configuration mixing, is a successful tool for describing the autoionization states of a rubidium atom in a wide range of collision energies and allowed us to obtain absolute values of excitation experimental cross-sections of $(4p^55s^2)^2P_{3/2,1/2}$ and $(4p^54d5s)^4P_{1/2,3/2,5/2}$ states.

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Теоретичні розрахунки електронного збудження найнижчих автоіонізаційних станів атома Rb

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Анотація

Мета. Значення перерізу автоіонізації та його енергетична залежність значною мірою визначаються збудженням та подальшим розпадом електронів найнижчих енергетичних станів. Нещодавно було отримано експериментальні дані про перерізи збудження найнижчого дублету атома рубідію $(4p^55s^2)^2P_{3/2,1/2}$ та квартету $(4p^54d5s)^4P_{1/2,3/2,5/2}$ автоіонізаційних станів, що сприяло їх теоретичним дослідженням.

Методи. Теоретичні розрахунки було проведено за допомогою універсального пакету програм «Гнучкий атомний код», який враховує релятивістську природу збудження складних атомів за допомогою гамільтоніана Дірака-Кулона. Радіальні орбіталі для основних релятивістських хвильових функцій було отримано шляхом розв'язання рівняння Дірака-Фока-Слейтера.

Результати. Подано порівняння експериментальних перерізів збудження для дублетних $(4p^5 5s^2)^2P_{3/2,1/2}$ та квартетних $(4p^5 4d5s)^4P_{1/2,3/2,5/2}$ автоіонізаційних станів з наявними теоретичними даними та нашими релятивістськими розрахунками. Представлено результати дослідження параметра R_0 відношення інтенсивностей для станів $^2P_{3/2}$ та $^2P_{1/2}$ конфігурації $4p^5 5s^2$. Показано, що наші розрахунки в наближенні спотворених хвиль добре описують експериментальні дані в області енергії вище 70 еВ. При малих енергіях зіткнення наші розрахунки якісно передбачають наявність порогового резонансного збудження; однак у енергетичній області 20–50 еВ лише метод R-матриці якісно описує складну природу збудження та розпаду найнижчих квартетних автоіонізаційних станів атома рубідію.

Висновки. Електронне збудження дублету $(4p^5 5s^2)^2P_{3/2,1/2}$ та квартету $(4p^5 4d5s)^4P_{1/2,3/2,5/2}$ автоіонізуючих станів атома рубідію в діапазоні енергій зіткнення від порогів збудження до 700 еВ було досліджено в термінах релятивістського наближення спотворених хвиль. Комплексний аналіз отриманих результатів з використанням наявних експериментальних та теоретичних даних показав, що апроксимація релятивістських спотворених хвиль з урахуванням конфігураційного змішування є відповідним інструментом для опису автоіонізаційних станів атома рубідію у широкому діапазоні енергій зіткнення. для отримання абсолютних значень експериментальних перерізів збудження

Ключові слова: атом, електронне збудження, автоіонізаційні стани, переріз збудження

Теоретические расчеты электронного возбуждения низких автоионизационных состояний атома Rb

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Аннотация

Цель. Значения сечения автоионизации и их энергетическая зависимость в значительной степени определяются возбуждением и последующим распадом электронов самых низких энергетических состояний. Недавно были получены экспериментальные данные о сечениях возбуждения самого низкого дублета атома рубидия $(4p^5 5s^2)^2P_{3/2,1/2}$ и квартета $(4p^5 4d5s)^4P_{1/2,3/2,5/2}$ автоионизационных состояний, что способствовало их теоретическим исследованиям.

Методы. Теоретические расчеты были произведены с помощью универсального пакета программ «Гибкий атомный код», учитывающего релятивистскую природу возбуждения сложных атомов с помощью гамильтониана Дирака-Кулона. Радиальные орбитали для основных релятивистских волновых функций были получены решением уравнения Дирака-Фока-Слейтера.

Результаты. Представлено сравнение экспериментальных сечений возбуждения для дублетных $(4p^5 5s^2)^2P_{3/2,1/2}$ и квартетных $(4p^5 4d5s)^4P_{1/2,3/2,5/2}$ автоионизационных состояний с имеющимися теоретическими данными и нашими релятивистскими расчетами. Представлены результаты исследования параметра R_0 относительно интенсивностей для состояний $^2P_{3/2}$ и $^2P_{1/2}$ конфигурации $4p^5 5s^2$. Показано, что наши расчеты в приближении искаженных волн хорошо описывают экспериментальные данные в области энергии выше 70 эВ. При малых энергиях столкновения наши расчеты отменно подразумевают наличие порогового резонансного возбуждения; однако в энергетической области 20–50 эВ только метод R-матрицы качественно описывает сложную природу возбуждения и распада самых низких квартетных автоионизационных состояний атома рубидия.

Выводы. Электронное возбуждение дублета $(4p^5 5s^2)^2P_{3/2,1/2}$ и квартета $(4p^5 4d5s)^4P_{1/2,3/2,5/2}$ автоионизирующих состояний атома рубидия в диапазоне энергий столкновения от порогов возбуждения до 700 эВ волн. Комплексный анализ полученных результатов с использованием имеющихся экспериментальных и теоретических данных показал, что аппроксимация искаженных релятивистских волн с учетом конфигурационного смешения является соответствующим инструментом для описания автоионизационных состояний атома рубидия в широком диапазоне энергий столкновения для получения абсолютных значений экспериментальных сечений возбуждения

Ключевые слова: атом, электронное возбуждение, автоионизационные состояния, сечение возбуждения