Near-threshold electron-impact excitation of the $(3p^5 4s4p)\,^4S_{3/2}$ quasimetastable state in potassium

A. A. Borovik, Jr.,[1] A. A. Borovik,[2] O. Zatsarinny,[3] and K. Bartschat[3]
[1]*Uzhgorod National University, 88000, Uzhgorod, Ukraine*
[2]*Institute of Electron Physics, Uzhgorod, 88017, Ukraine*
[3]*Department of Physics and Astronomy, Drake University, Des Moines, Iowa 50311, USA*
(Received 25 January 2006; published 1 June 2006)

Electron-impact excitation of the $(3p^5 4s4p)\,^4S$ quasimetastable level in potassium has been investigated both experimentally and theoretically for incident energies up to 3 eV above the excitation threshold. The ejected-electron excitation function measured with an energy resolution of 0.25 eV suggests the presence of several strong resonances just above threshold. Satisfactory agreement with the excitation cross section obtained from a sophisticated *B*-spline *R*-matrix model with nonorthogonal orbitals supports the importance of K^- resonances predominantly of the $(3p^5 4s4p^2)$ configuration. Good agreement between theory and experiment is also obtained for the optical excitation function measured earlier with a lower energy resolution of ≈ 1.2 eV. The branching ratios for decay of the $(3p^5 4s4p)\,^4S_{3/2}$ level into the electron emission and the optical channels were obtained as 0.16 and 0.69, respectively.

DOI: 10.1103/PhysRevA.73.062701 PACS number(s): 32.80.Dz, 34.80.Dp

One of the most interesting peculiarities in the excitation of the outer p^6 subshells in heavy alkali metals (K, Rb, Cs) is the presence of a subclass of quartet levels, which retain metastability against autoionization [1,2]. In a purely nonrelativistic (*LS* coupling) description, these quartet levels are prohibited to decay via either autoionization or emission of radiation. Relativistic effects, however, allow for the mixing of the quartet levels (except for that with the highest total electronic angular momentum *J*) with doublet levels of the same *J*. Hence both decay paths for these "quasimetastable" atoms become open, often with significant radiation yield, while the probability for autoionization remains small.

In potassium atoms, three low-lying quasimetastable levels are known, namely, $(3p^5 3d4s)\,^4P_{5/2}$ at 19.86 eV, $(3p^5 4s4p)\,^4S_{3/2}$ at 20.02 eV, and $(3p^5 3d4s)\,^4F_{3/2}$ at 20.59 eV [2,3]. For all these levels, the decay in both radiative and electron emission (autoionization) channels has been observed earlier [2,4,5]. These data show that the emission lines corresponding to the radiative decay dominate the neutral spectrum of potassium atoms, while the lines in the ejected-electron spectra are weak. This is the principal reason why, up to date, electron-impact excitation of the $(3p^5 3d4s)\,^4P_{5/2}$ and $(3p^5 4s4p)\,^4S_{3/2}$ levels has only been observed by detection of photon emission in the extreme ultraviolet region [6]. Despite a poor energy resolution ($\Delta E \approx 1.2$ eV), the latter data suggested the importance of resonances in the near-threshold impact energy regime.

In a recent joint experimental and theoretical study, we successfully applied the ejected-electron spectroscopy technique to obtain high-resolution ejected-electron excitation functions for the $(3p^5 4s^2)\,^2P_{3/2,1/2}$ levels in potassium [7]. When investigating the quasimetastable levels, however, significant problems can be expected in such measurements due to the overlap of weak lines and the "wings" of strong neighboring lines. Indeed, an analysis of earlier ejected-electron spectra [8] shows that this situation exists for the $(3p^5 3d4s)\,^4P_{5/2}$ line, which is strongly overlapped by the dominant $^4P_{3/2}$ component separated by less than 0.07 eV, as well as for the $(3p^5 3d4s)\,^4F_{3/2}$ line lying in one of the most crowded spectral regions between 20.55 and 20.77 eV. The energy position of the $(3p^5 4s4p)\,^4S_{3/2}$ line, however, is much more suitable from an experimental point of view, since it is separated from the nearest neighboring lines by about 0.15 eV on either side. Hence, we selected the $(3p^5 4s4p)\,^4S_{3/2}$ level as the object for the present benchmark comparison between high-resolution experimental data and predictions from a sophisticated close-coupling-type model.

The apparatus and the measuring procedure used in the present work were described earlier [7]. The ejected-electron excitation function for the $^4S_{3/2}$ level was measured with an energy width of 0.25 eV in the incident electron beam, over an impact energy range from the excitation threshold of 20.02 eV [3] up to 23 eV. We limited the measurements to this maximum energy value due to the rising intensities of the $(3p^5 3d4s)\,^4P_{3/2,5/2}$ and $(3p^5[3d4s]^3P)\,^2P_{1/2,3/2}$ neighboring lines and their resulting overlap with the $^4S_{3/2}$ line. Each point in the excitation function was obtained as the mean value of the data obtained from three independent measurements. The relative uncertainty, after accounting for fluctuations in the experimental conditions, reached approximately 25% for most of the data, with some larger uncertainties occurring near minima in the observed signal.

The numerical calculations were performed with a newly developed *B*-spline atomic *R*-matrix (close-coupling) code [9]. Details of the method can also be found in Refs. [10,11]. The key feature of the approach is to significantly improve the target description by employing compact configuration-interaction expansions involving nonorthogonal sets of term-dependent one-electron orbitals for different target states. In the present calculations, for example, we used different 3*s* and 3*p* core orbitals for the ground and the core-excited states. This procedure allows us to account for the important core-relaxation effects essentially to full extent. The present scattering model included 58 fine-structure target states, namely, all those that could be constructed from the $3p^6 4s$, $3p^6 4p$, $3p^5 4s^2$, $3p^5 3d4s$, $3p^5 4s4p$, and $3p^5 4s5s$ configura-

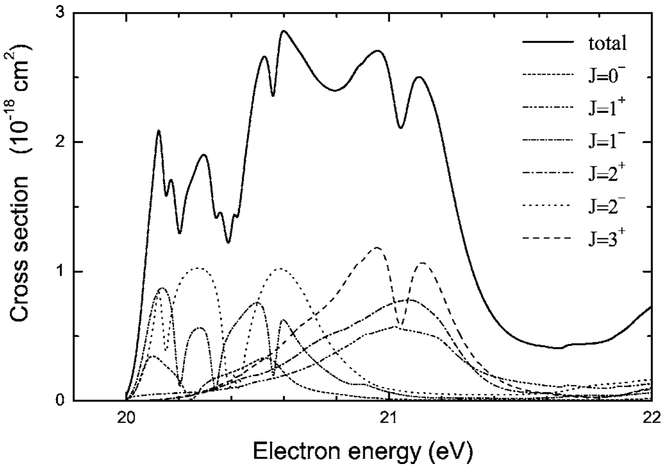

FIG. 1. Partial-wave decomposition of the BSR-58 total excitation cross section for the $(3p^5 4s4p)\,^4S_{3/2}$ level in potassium.

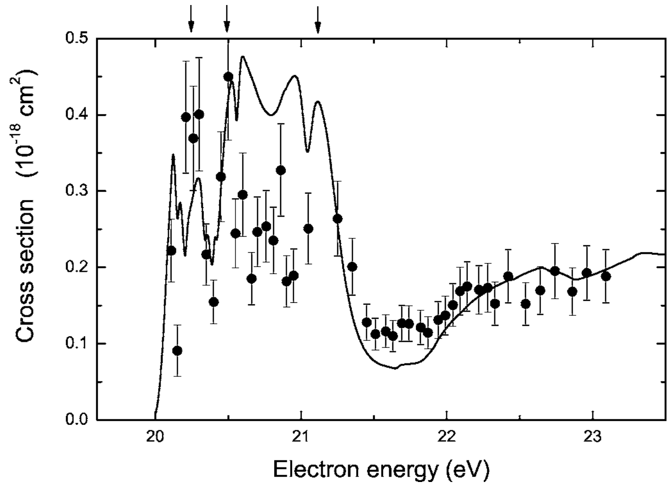

FIG. 2. Electron-impact excitation cross section for the $(3p^5 4s4p)\,^4S_{3/2}$ level, as observed in the ejected-electron channel. The solid circles represent the measured data, normalized to the BSR-58 predictions (solid line) for incident energies between 22 and 23 eV. Note that the theoretical results were multiplied by 0.16 to account for the autoionization yield. The arrows on top of the frame mark the clearly identifiable structures in the experimental data (see text).

tions, plus a few selected states of the $3p^5 4p^2$ and $3p^5 4s4d$ configurations, namely, those that exhibit strong configuration interaction with the previously mentioned states. The valence orbitals were obtained from term-averaged Hartree-Fock calculations for a given configuration, and hence all orbitals include term-dependent effects. Finally, relativistic effects were accounted for by including all one-electron terms of the Breit-Pauli Hamiltonian. This model will be labeled as BSR-58 below.

Figure 1 exhibits the calculated total cross section and its partial-wave decomposition in the low-energy region from threshold to 22 eV. The prominent resonance structure observed just above the excitation threshold originates from the dominant contributions of the six partial waves J^π indicated in the legend. These partial waves correspond to the scattering of incident electrons with orbital angular momenta $\ell = 1,2$. Note that the odd-parity symmetries $J = 0^-, 1^-$, and 2^- contribute mainly in the near-threshold region below 20.8 eV, and these contributions are strongly affected by a narrow resonance structure. On the other hand, the even-parity partial cross sections from the $J = 1^+$, 2^+, and 3^+ symmetries show maxima at slightly higher incident energies around 21 eV, and only the $J = 3^+$ contribution exhibits a broad resonance feature. An analysis of the R-matrix poles in this region shows that all odd-parity resonances are predominantly of the $(3p^5 4s4p^2)$ configuration.

The measured cross section for electron-impact excitation of the $(3p^5 4s4p)\,^4S_{3/2}$ state with subsequent decay by electron emission is presented in Fig. 2. The experimental data were visually normalized to the theoretical predictions in the energy range between 22 and 23 eV, where the agreement between the measured and predicted energy dependence is good. According to our theoretical estimates, the total decay probability of the $(3p^5 4s4p)\,^4S_{3/2}$ state is approximately $6 \times 10^6\ \mathrm{s}^{-1}$, with a branching ratio of 0.16 for the autoionizing path. The theoretical data plotted in Fig. 2 have thus been obtained by multiplying the calculated total excitation cross sections by this probability for autoionization.

As might be expected from the theoretical predictions shown in Fig. 1, a remarkable energy dependence is evident in the measured cross section. These data clearly support the presence of resonances, possibly smoothed out by the limited energy resolution of the present experimental setup. Nevertheless, three resonance features, observed at 20.25, 20.50, and 21.16 eV (marked by arrows in Fig. 2), match up satisfactorily with the calculated structures around these energies. The large value of the cross section observed in the first point of the experimental excitation function likely reflects the presence of several strong narrow resonances located up to 0.2 eV above the excitation threshold (see partial waves $J = 0^-, 1^-$, and 2^- in Fig. 1).

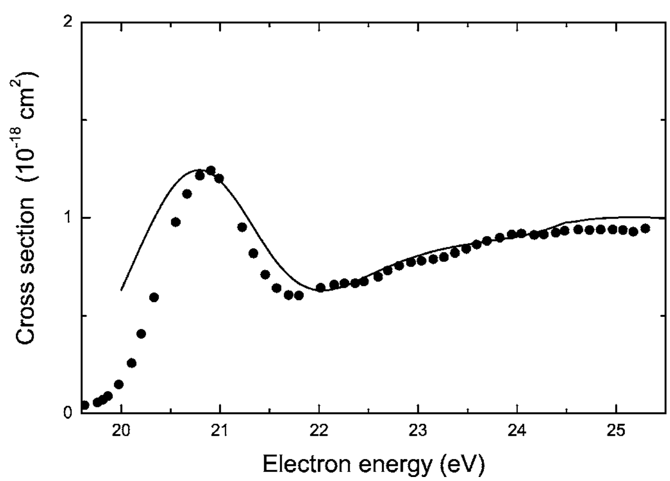

FIG. 3. Emission cross section for the $(3p^5 4s4p)\,^4S_{3/2} \rightarrow (3p^6 4p)\,^2P_{3/2}$ transition. The experimental data of Bogachev and Marushka (see Ref. [6]) (solid circles) were visually normalized to the BSR-58 predictions. The latter results were convoluted with a Gaussian of 1.2 eV [full width at half maximum (FWHM)] and multiplied by the branching ratio of 0.69 for radiative decay.

Finally, let us consider the radiative emission from the $(3p^5 4s4p)\,^4S_{3/2}$ level. Figure 3 exhibits the optical excitation function for the $(3p^5 4s4p)\,^4S_{3/2} \rightarrow (3p^6 4p)\,^2P_{3/2}$ ($\lambda = 67.4$ nm) transition measured earlier with an energy resolution of 1.2 eV [6]. The experimental data were made absolute by normalizing to the BSR-58 total excitation cross section multiplied by the theoretical fluorescence yield factor of 0.69. We note good agreement between experiment and theory regarding the energy dependence of the excitation function over the entire energy regime. In particular, our calculation confirms the distinctive near-threshold maximum, which is the combined result of contributions from many negative-ion resonances.

In conclusion, the total excitation cross section of the $(3p^5 4s4p)\,^4S_{3/2}$ quasimetastable level in potassium has been investigated both experimentally and theoretically for incident electron energies up to 3 eV above the excitation threshold. In both the theoretical and the experimental energy dependence of the cross sections we found a complicated structure due to core-excited K^- resonances predominantly of the $(3p^5 4s4p^2)$ configuration. In order to resolve the remaining discrepancies between experiment and theory, even larger calculations may need to performed. Unfortunately, the convergence of the close-coupling expansion with the number of states is expected to be slow [12]. Hence, given the size of the present experimental uncertainties and the significant computational resources required to increase the size of the close-coupling expansion substantially, we decided not to further pursue the convergence issue at the present time.

This work was supported, in part, by INTAS under Grant No. 03-51-4706 (A.A.B.) and by the United States National Science Foundation under Grants No. PHY-0244470 (K.B.) and PHY-0311161 (O.Z. and K.B.).

[1] S. E. Harris, D. J. Walker, R. G. Caro, A. J. Mendelsohn, and R. D. Cowan, Opt. Lett. **9**, 168 (1984).

[2] A. J. Mendelsohn, C. P. J. Barty, M. H. Sher, J. F. Young, and S. E. Harris, Phys. Rev. A **35**, 2095 (1987).

[3] M. W. D. Mansfield and T. W. Ottley, Proc. R. Soc. London, Ser. A **365**, 413 (1979).

[4] G. Kavei, T. W. Ottley, V. Pejev, and K. J. Ross, J. Phys. B **10**, 2923 (1977).

[5] I. S. Aleksakhin, G. G. Bogachev, I. P. Zapesochny, and S. Yu Ugrin, Sov. Phys. JETP **53**, 1140 (1981).

[6] G. G. Bogachev and Ya. I. Marushka, in Book of Abstracts of the 19th International Conference on the Physics of Electronic and Atomic Collisions, edited by J. B. A. Mitchell, J. W. McConkey, and C. E. Brion (unpublished), p. 483.

[7] A. A. Borovik, A. N. Grum-Grzhimailo, K. Bartschat, and O. Zatsarinny, J. Phys. B **38**, 1081 (2005).

[8] M. J. Evrij, A. A. Borovik, Jr., L. L. Shimon, J. E. Kontros, and A. A. Borovik, Nucl. Instrum. Methods Phys. Res. B **233**, 280 (2005).

[9] O. Zatsarinny, Comput. Phys. Commun. **174**, 273 (2006).

[10] O. Zatsarinny and C. Froese Fischer, J. Phys. B **33**, 313 (2000).

[11] O. Zatsarinny and K. Bartschat, J. Phys. B **37**, 4693 (2004).

[12] A. N. Grum-Grzhimailo and K. Bartschat, J. Phys. B **33**, 1843 (2000).