J. Phys. B: At. Mol. Opt. Phys. **32** (1999) 4547–4554. Printed in the UK PII: S0953-4075(99)05454-1

# Electron-impact excitation cross sections of $K^*(3p^5 4s^2\ ^2P_{3/2}, {}^2P_{1/2})$ autoionizing states: strong fine-structure dependence near threshold

B Feuerstein, A N Grum-Grzhimailo† and W Mehlhorn
Fakultät für Physik, Universität Freiburg, D-79104 Freiburg, Germany

Received 24 June 1999

**Abstract.** The electron-impact cross sections of the inner-shell excited autoionizing states $K^*(3p^5 4s^2\ ^2P_{3/2})$ and $K^*(3p^5 4s^2\ ^2P_{1/2})$ were measured for the incident energy ranges from threshold up to 1 keV and up to 37.2 eV, respectively. A strong negative-ion resonance structure was found in the excitation cross section of the $^2P_{3/2}$ state close to the threshold, whereas the excitation function of the $^2P_{1/2}$ state is rather smooth. For impact energies below 40 eV the cross section ratio $R$ of the fine-structure components shows a substantial energy-dependent deviation from the statistical value $R = 2$. The present experimental values are compared with recent theoretical results obtained in the distorted-wave Born approximation.

## 1. Introduction

The formation of negative-ion resonances is a well known phenomenon in electron–atom scattering processes (see, e.g., the review by Buckman and Clark 1994). In inelastic scattering processes near threshold the outgoing low-energy electron can be captured by the atom into a short-lived negative charged compound state. These states manifest themselves as resonance structures in the corresponding excitation cross sections. Recently, it was shown experimentally and theoretically that negative-ion resonances play an important role in the near-threshold inner-shell excitation of the $2p^5 3s^2\ ^2P$ autoionizing state (AIS) in sodium (Feuerstein *et al* 1998). Resonance structures in the excitation functions for other AIS in alkali atoms have been observed repeatedly (Feldman and Novick 1967, Pejčev and Ross 1977, Borovik *et al* 1993, Rojas *et al* 1995, Bogashev and Marushka 1995, Borovik and Krasilinec 1999). In the work of Borovik *et al* (1993) a near-threshold resonance structure had been found for the intensity $I(\vartheta)$ of autoionization electrons from the decay of $K^*(3p^5 4s^2\ ^2P_{3/2})$ measured at an emission angle $\vartheta = 75^\circ$. The intensity $I(\vartheta)$ then depends on the excitation cross section of the AIS as well as on its alignment via the anisotropic emission (see equation (2) below).

In a previous work (Matterstock *et al* 1995) the alignment of the $K^*(3p^5 4s^2\ ^2P_{3/2})$ AIS as well as the cross section ratio $R = \sigma_{3/2}/\sigma_{1/2}$ of the fine-structure components $3p^5 4s^2\ ^2P_{3/2}$ and $^2P_{1/2}$ were measured for impact energies in the range 31.4–500 eV. The cross section ratio $R$ showed a small deviation from the statistical value of 2 at high impact energies ($R = 2.05(1)$); below 100 eV the cross section ratio is energy dependent, leading to a ratio $R = 1.92(2)$ at 31.4 eV. These results indicate the influence of spin–orbit effects on the atomic structure as

† Permanent address: Institute of Nuclear Physics, Moscow State University, 119899 Moscow, Russia.

0953-4075/99/184547+08$30.00  

well as on the dynamics of the excitation process. In continuation of this investigation and with the purpose of studying the near-threshold negative-ion resonance region in more detail, we have now measured the electron-impact excitation cross section of the $K^*(3p^5 4s^2\ ^2P_{3/2})$ AIS for impact energies $E_0$ from threshold (18.7 eV) to 1000 eV, and the cross section of the $K^*(3p^5 4s^2\ ^2P_{1/2})$ AIS for impact energies $E_0 = 19.2$–$37.2$ eV.

## 2. Experiment

The cross section for excitation of $K^*(3p^5 4s^2\ ^2P_{3/2}, {}^2P_{1/2})$ by electron impact

$$e^-(E_0) + K(3p^6 4s\ ^2S_{1/2}) \longrightarrow K^*(3p^5 4s^2\ ^2P_{3/2}, {}^2P_{1/2}) + e^-_{sc} \tag{1a}$$

which decay under emission of an autoionization electron $e^-_A$ into the ground state of $K^+$

$$K^*(3p^5 4s^2\ ^2P_{3/2}, {}^2P_{1/2}) \longrightarrow K^+(3p^6\ ^1S_0) + e^-_A \tag{1b}$$

is measured via the intensity $I_A$ of autoionization electrons at the emission angle $\vartheta = 54.7^\circ$ relative to the direction of the incident electron beam. The intensity $I_A$ is given by (Cleff and Mehlhorn *et al* 1974, Berezhko and Kabachnik 1977)

$$I_A(E_0, \vartheta) = \sigma(E_0)(1 + \mathcal{A}_{20}(E_0)\,\alpha_2 P_2(\cos\vartheta))D. \tag{2}$$

Here, $\mathcal{A}_{20}$ is the alignment parameter of the AIS and $\alpha_2$ is the decay parameter, the latter has the value $-1$ for the decay (1*b*). $P_2(\cos\vartheta)$ is the second Legendre polynomial which is zero at $\vartheta = 54.7^\circ$. Thus, the detected intensity of autoionization electrons does not depend on the alignment $\mathcal{A}_{20}$ of the AIS. $D$ includes the intensity of incident electrons, the target density and the total detection efficiency. The measured intensities $I_A(E_0)$ for impact energies $E_0$ were normalized to the corresponding intensity $I_N$ for a fixed impact energy of 500 eV in order to determine the relative cross section values $\sigma(E_0)/\sigma(500\ \text{eV})$.

A detailed description of the experimental method and of the apparatus used in the present investigation is given by Feuerstein *et al* (1998). For the incident electron beams we used two different electron guns. These guns are mounted on a rotatable platform for alternating measurements of cross section spectra and normalization spectra. One electron gun is used at a fixed energy of 500 eV for normalization, while the other electron gun is used at various incident energies $E_0$ for cross section measurements. We choose 500 eV for normalization, because both electron guns work well at this energy and therefore the consistency of both measurements could be checked. The typical operation temperature of the K vapour target cell was about 170 °C, which corresponds to a target density of $\sim 5 \times 10^{13}$ cm$^{-3}$.

The impact energy $E_0$ of the primary electrons was determined by comparing the energy of the elastically scattered electrons to the energy $E_A$ of the autoionization electrons from the decay of the $^2P_{3/2}$ state. The latter energy is known to be 14.38 eV (Kavei *et al* 1977). For the measurements in the threshold region the energy distribution of the incident electrons was optimized to 700–800 meV (FWHM) by reduction of the filament temperature. The FWHM was measured via the elastically scattered electrons.

An example for the doublet lines measured at an impact energy $E_0 = 19.7$ eV is shown in figure 1. The full line is a least-squares fit to the experimental spectrum, the components of which are plotted below. These components are due to the decay of the diagram states $^2P_{3/2}$ and $^2P_{1/2}$ (full curves) and of three satellite states with unknown configuration (dotted curves); the satellite lines have also been found by Matterstock *et al* (1995). The asymmetry of the lineshapes is due to the post-collision interaction (PCI) between the low-energy scattered electron (in the case of figure 1 the energy of the scattered electron is $E_1 = 1$ eV) and the autoionization electron (Read 1977, Ogurtsov 1983, Kuchiev and Sheinerman 1988).

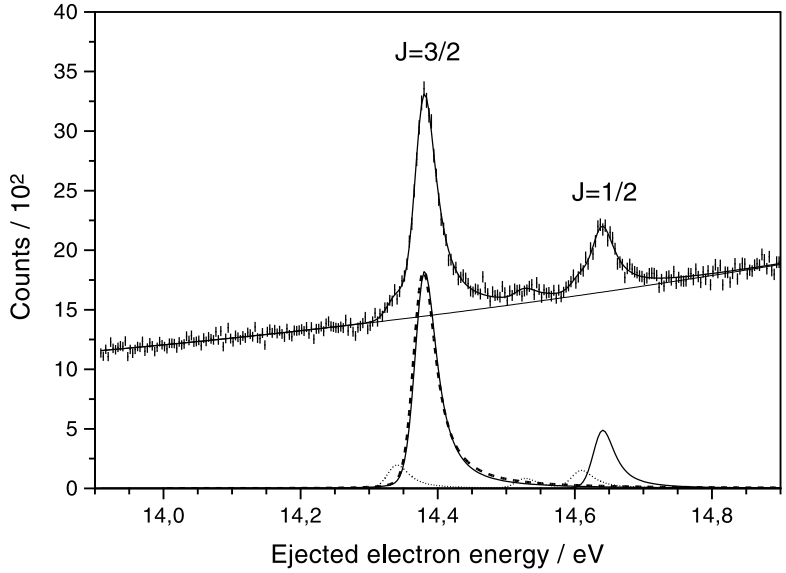


**Figure 1.** Autoionization doublet of the decay $K^*(3p^5 4s^2\ ^2P_{3/2}, ^2P_{1/2}) \rightarrow K^+(3p^6\ ^1S_0) + e_A^-$, taken at an impact energy of $E_0 = 19.7$ eV (1 eV above the threshold of the $^2P_{3/2}$ state) for an emission angle $\vartheta = 54.7^\circ$. The full line represents a computer fit to the spectrum. The corresponding components are shown as full curves ($^2P_J$ diagram states) and as dotted curves (satellite states), whereas the broken curve is a PCI function convolved with the Gaussian apparatus function with FWHM = 25 meV (for details see text).

Using equation (5) of Ogurtsov (1983), we calculated the PCI lineshape for the $^2P_{3/2}$ AIS for $E_1 = 1$ eV and a Lorentzian width of $\Gamma = 5.2$ meV (Zatsarinny 1999) and convolved it with the apparatus function (a Gaussian function with FWHM = 25 meV). This result is plotted as a broken curve in figure 1. It should be noted that no effect of Fano interference (Fano 1961) on the lineshape was observed. From an analysis of the lineshape by using a Fano profile with different $q$ parameters convolved with the PCI function and the apparatus function we conclude that the Fano parameter $q$ must have a value $|q| \gtrsim 20$.

The relative cross section values obtained from the experiment were put on an absolute scale by normalization of the intensity $I_N$ to a theoretical value for the cross section at 500 eV (Feuerstein *et al* 1998). For this we used a value obtained within the plane-wave Born approximation (PWBA) based on the same wavefunctions as in the previous PWBA calculation for the alignment (Matterstock *et al* 1995): $\sigma(^2P_{3/2}, 500\ \text{eV}) = 2.56 \times 10^{-18}\ \text{cm}^2$. At that high impact energy (26.7 times the threshold energy) PWBA gives reliable cross sections provided that good atomic wavefunctions are used in the calculation. A main systematic error in the absolute value of the cross section $\sigma(^2P_{3/2}, 500\ \text{eV})$ may come from the single-configuration Hartree–Fock description of the potassium ground state in the PWBA calculation in contrast to the very sophisticated treatment of the autoionizing state (Matterstock *et al* 1995). Core-polarization effects are known to influence strongly the oscillator strengths for valence electron transitions in potassium and heavier alkalis (for example, Migdalek and Kim 1998). The core-excited components of the wavefunction which are responsible for the core-polarization effects (e.g. $3p^4 3d^2$ for potassium) show noticeable expansion coefficients in the ground state wavefunction (Zatsarinny 1999) and should be taken into account in accurate calculations. The non-orthogonality of the electron orbitals before and after the excitation can give an additional

**Table 1.** Experimental values of the cross sections $\sigma_{3/2}$ and $\sigma_{1/2}$ and of the cross section ratio $R = \sigma_{3/2}/\sigma_{1/2}$ of the fine-structure states $^2P_{3/2}$ and $^2P_{1/2}$ of $K^*(3p^5 4s^2)$ for electron-impact excitation at incident energies $E_0$.

| $E_0$ (eV) | $\sigma_{3/2}$ ($10^{-18}$ cm$^2$) | $\sigma_{1/2}$ ($10^{-18}$ cm$^2$) | $R$ |
|---|---|---|---|
| 18.2 | 1.07(24) | | |
| 18.5 | 0.81(23) | | |
| 18.7 | 5.11(45) | | |
| 19.0 | 10.6(8) | | |
| 19.2 | 9.9(9) | 1.73(24) | 5.7(6) |
| 19.5 | 14.8(12) | 2.52(25) | 5.87(34) |
| 19.7 | 14.6(21) | 4.2(6) | 3.46(20) |
| 20.0 | 6.1(6) | 2.35(27) | 2.58(17) |
| 20.5 | 5.5(6) | 2.67(44) | 2.05(25) |
| 21.5 | 5.9(5) | 2.98(31) | 1.98(13) |
| 21.7 | 6.2(5) | 3.07(30) | 2.01(12) |
| 22.2 | 6.2(6) | 2.86(33) | 2.17(13) |
| 23.2 | 5.25(40) | 2.77(26) | 1.90(10) |
| 24.3 | 3.82(34) | 2.56(31) | 1.49(12) |
| 25.3 | 3.49(33) | 2.30(29) | 1.52(12) |
| 26.3 | 3.22(32) | 1.87(23) | 1.72(12) |
| 27.2 | 3.76(31) | 2.28(23) | 1.65(10) |
| 28.1 | 3.28(41) | 1.70(23) | 1.93(9) |
| 29.1 | 3.13(24) | 1.78(16) | 1.76(8) |
| 30.1 | 3.23(27) | 1.79(17) | 1.80(8) |
| 32.2 | 3.73(20) | 2.18(14) | 1.71(6) |
| 37.2 | 3.22(27) | 1.61(15) | 2.00(8) |
| 42.2 | 3.04(28) | | |
| 50 | 3.55(13) | | |
| 60 | 4.42(20) | | |
| 80 | 5.32(10) | | |
| 100 | 5.12(15) | | |
| 150 | 4.88(13) | | |
| 200 | 4.48(18) | | |
| 300 | 3.53(10) | | |
| 500 | 2.56[a] | | |
| 750 | 1.89(5) | | |
| 1000 | 1.51(5) | | |

[a] Normalized to PWBA value (see text).

inaccuracy; this effect was found to be 6–7% in the case of $Na^*(2p^5 3s^2\,^2P)$ (Feuerstein *et al* 1998).

The results for the cross sections $\sigma_{3/2}$ and $\sigma_{1/2}$ of AIS $K^*(3p^5 4s^2\,^2P_{3/2}$ and $^2P_{1/2})$ and for the cross section ratio $R = \sigma_{3/2}/\sigma_{1/2}$ are listed in table 1 and are plotted in figures 2–4.

## 3. Results and discussion

Figure 2 shows the excitation function of $K^*(3p^5 4s^2\,^2P_{3/2})$ for the impact energy range from threshold up to 1 keV. The present experimental values are compared with theoretical curves based on PWBA and distorted-wave Born approximation (DWBA) models (Matterstock *et al* 1995, Kaur and Srivastava 1999) and with the experimental results from a previous work of Borovik *et al* (1993). Note that the latter cross section values were measured at an emission angle of $\vartheta = 75^\circ$ and, hence, depend on the alignment of the autoionizing state

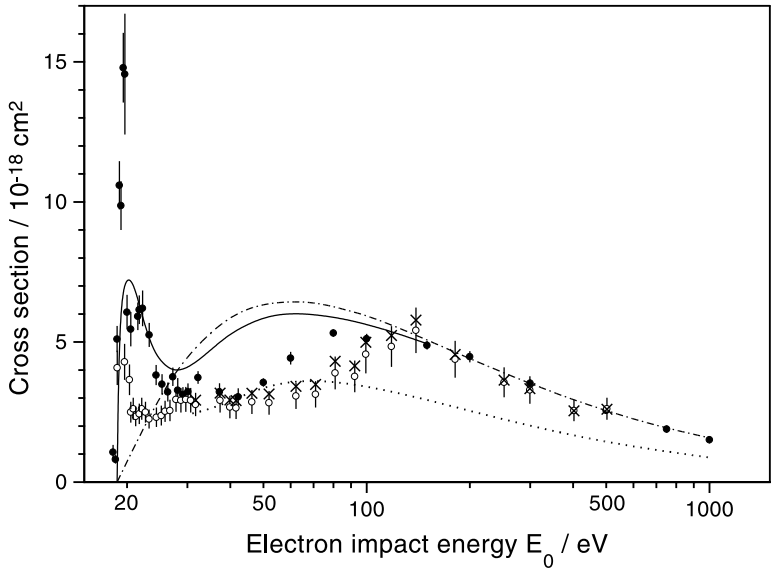


**Figure 2.** Excitation function of $K^*(3p^5 4s^2\ ^2P_{3/2})$ for electron impact. Experiment: ●, this work; ○, Borovik *et al* (1993) (measured at $\vartheta = 75^\circ$); ×, calculated values for $\vartheta = 54.7^\circ$ using the alignment parameters from Matterstock *et al* (1995). Theory: — · —, PWBA; ——, DWBA (this work); · · · · · ·, RDWBA (Kaur and Srivastava 1999).

(see equation (2)). By using the known alignment values from Matterstock *et al* (1995) in the impact energy region $E_0 = 30$–$500$ eV, we calculated the corresponding cross sections for an emission angle of $\vartheta = 54.7^\circ$ (shown as crosses in figure 2). The excitation function shows a broad maximum, typical for dipole-allowed excitations, around 100 eV and a strong resonance structure near threshold. Both features have also been observed by Borovik *et al* (1993), although the resonance structure is found to be much stronger in the present investigation. This shape of the excitation function is similar to those obtained for the $5p^5 6s^2\ ^2P_{3/2}$ AIS in caesium (Pejčev and Ross 1977) and for the $2p^5 3s^2\ ^2P$ AIS in sodium (Feuerstein *et al* 1998).

At intermediate impact energies (30–100 eV) the experiment gives a significantly different shape for the excitation function compared to the theoretical predictions based on PWBA and DWBA models. A similar effect has been observed for the electron-impact excitation of $Na^*(2p^5 3s^2\ ^2P)$ (Feuerstein *et al* 1998). In this case the reduction of cross sections was explained as a loss of flux due to other open channels. The importance of channel coupling for the collision dynamics at intermediate impact energies was also demonstrated by recent studies of the collision-induced alignment of $Na^*(2p^5 3s^2\ ^2P_{3/2})$ (Feuerstein *et al* 1999). Another possible source for the disagreement in shape for the excitation function of $K^*(3p^5 4s^2\ ^2P_{3/2})$ is a lack of core-polarization effects in the ground state, as has been discussed above.

The most interesting feature of the excitation function is the prominent resonance structure close to the threshold. Figure 3 shows the result for the cross section values of the fine-structure components $K^*(3p^5 4s^2\ ^2P_{3/2}, ^2P_{1/2})$ in more detail at low impact energies. The $^2P_{3/2}$ excitation function exhibits two structures, a sharp resonance at 19.5 eV and a broader structure at 22 eV. The latter may consist of several overlapping resonances which are not resolved due to the finite energy spread ($\simeq 0.75$ eV) of the incident electrons. Since the experimental width of the resonance at 19.5 eV is close to this energy spread, one could conclude that the natural width of the resonance is smaller than the observed width. In any case, the true resonance peak will

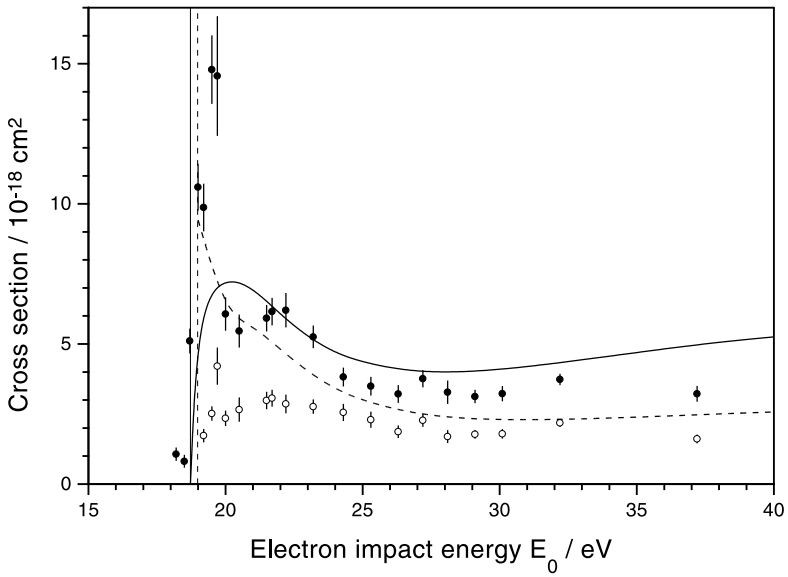


**Figure 3.** Cross sections of the fine-structure components $^2P_{3/2}$ and $^2P_{1/2}$ of $K^*(3p^5 4s^2\ ^2P)$ at low impact energies. Experiment (this work): ●, $J = \frac{3}{2}$; ○, $J = \frac{1}{2}$. Theory (DWBA, this work): ——, $J = \frac{3}{2}$; – – –, $J = \frac{1}{2}$. Thresholds are shown as a vertical full line (18.72 eV for $J = \frac{3}{2}$) and a vertical broken line (18.98 eV for $J = \frac{1}{2}$).

be flattened down and the measured cross section is a low limit of the true cross section. In contrast to the $^2P_{3/2}$ state the excitation function of the $^2P_{1/2}$ state is rather smooth.

In figure 3 theoretical curves are shown for both fine-structure components based on the DWBA model with intermediate coupling wavefunctions (Matterstock *et al* 1995) and with an optical potential leading to curve 7 of figure 3 of Matterstock *et al* (1995). The DWBA is not reliable at low energies, although it can sometimes reproduce resonance structures in the electron–atom excitation cross sections near the threshold (Bubelev and Grum-Grzhimailo 1990). The broad resonance structure of the $^2P_{3/2}$ AIS near threshold in figure 3 in the DWBA curve is due to a sharp maximum in the exchange amplitude combined with the shape resonance in the direct amplitude (Borovik *et al* 1993). The disagreement between the theoretical predictions and the experimental results in the resonance region below 24 eV calls for more sophisticated theoretical models, e.g. *R*-matrix (close-coupling) calculations, which have been successfully applied recently for the electron-impact excitation of $Na^*(2p^5 3s^2\ ^2P)$ (Feuerstein *et al* 1998).

In figure 4 we present the cross section ratio $R = \sigma_{3/2}/\sigma_{1/2}$ of the fine-structure components in extension of the previously given values by Matterstock *et al* (1995) down to threshold and compare it with theoretical curves based on DWBA models (Matterstock *et al* 1995, Kaur and Srivastava 1999). The ratio $R$ is shown as a function of the electron-impact energy in threshold units which allows a direct comparison with previous experimental and theoretical results for $Na^*(2p^5 3s^2\ ^2P_{3/2}, ^2P_{1/2})$ (Feuerstein *et al* 1999). In the latter case the ratio is close to the statistical value of $R = 2$ except for the resonance region near threshold, where the ratio exhibits some oscillations and a sharp increase at threshold. This behaviour can be explained kinematically within the $LS$-coupling approximation by simply introducing a fine-structure splitting of the excitation thresholds (model LS2 from Feuerstein *et al* (1999)). In

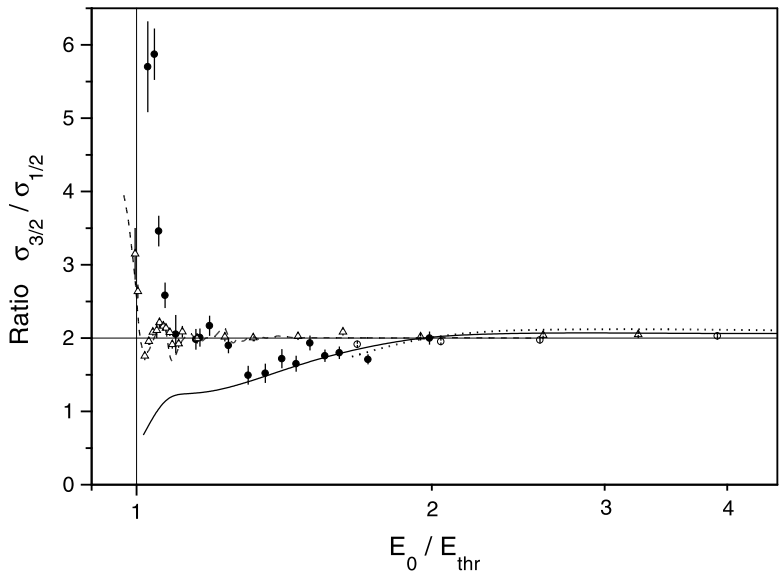


**Figure 4.** Cross section ratio $R = \sigma(\frac{3}{2})/\sigma(\frac{1}{2})$ of the fine-structure components $^2P_{3/2}$ and $^2P_{1/2}$ of $K^*(3p^5 4s^2\ ^2P)$ and $Na^*(2p^5 3s^2\ ^2P)$ as a function of electron-impact energy in threshold units. Potassium: experiment: ●, this work; ○, Matterstock *et al* (1995). Theory: ——, DWBA (curve number 3 of figure 4 from Matterstock *et al* (1995) is extended to lower energies); · · · · · ·, RDWBA (Kaur and Srivastava 1999). Sodium (Feuerstein *et al* 1999): △, experiment; – – –, theory (*R*-matrix, model LS2).

contrast, for potassium the energy dependence of the ratio is much stronger and is even present up to impact energies of two threshold units. This dynamical fine-structure dependence is well reproduced by the DWBA calculations (Matterstock *et al* 1995, Kaur and Srivastava 1999) for impact energies $E > 24$ eV ($1.3E_{\rm thr}$). The remaining discrepancy below 24 eV seems to be caused by the fact that the DWBA approach cannot reproduce the near-threshold negative-ion resonances. *R*-matrix calculations are planned to give a deeper insight into the dynamics of the excitation process at low energies.

## 4. Conclusions

We measured the relative excitation cross sections of the autoionizing states $K^*(3p^5 4s^2\ ^2P_{3/2})$ and $K^*(3p^5 4s^2\ ^2P_{1/2})$ for electron impact in the range of incident energies from threshold up to 1 keV and from 19.2 up to 37.2 eV, respectively. Absolute cross section values were obtained by normalizing the experimental result at 500 eV to a PWBA calculation. Our measurements have revealed a strong fine-structure dependence of the shape of the excitation function at low energies which yields a substantial energy-dependent deviation of the cross section ratio $R$ of the fine-structure components from the statistical value $R = 2$. The shape of the excitation function $\sigma(^2P_{3/2}, E_0)$ at intermediate energies shows a loss of cross section compared to theoretical predictions based on simple perturbative models. The similarity to the case of $Na^*(2p^5 3s^2\ ^2P)$ (Feuerstein *et al* 1998) emphasizes the general importance of channel coupling for the electron-impact excitation of autoionizing states in alkali atoms at low and intermediate energies.

**Acknowledgments**

The authors are grateful to O I Zatsarinny for collaboration. This work is part of the joint program 'Dynamics of Autoionizing and Auger States of Alkali Atoms Excited by Electron Impact: Experiment and Theory', supported by the Deutsche Forschungsgemeinschaft and by the Russian Foundation for Basic Research. It is also supported by the Deutsche Forschungsgemeinschaft via the Sonderforschungsbereich 276 'Correlated Dynamics of Highly Excited Atomic and Molecular Systems'. ANG gratefully acknowledges the hospitality of the Albert-Ludwigs-Universität Freiburg and support from the Foundation 'Universities of Russia' under grant no 5340.

## References

Berezhko E G and Kabachnik N M 1977 *J. Phys. B: At. Mol. Phys.* **10** 2467
Bogachev G G and Marushka Ya I 1995 *Proc. XIXth Int. Conf. on the Physics of Electronic and Atomic Collisions (Whistler, NY)* ed J B Mitchell *et al* (Amsterdam: North-Holland) p 483
Borovik A A, Grum-Grzhimailo A N and Zatsarinny O I 1993 *Proc. XVIIIth Int. Conf. on the Physics of Electronic and Atomic Collisions (Aarhus)* ed T Anderson *et al* (Amsterdam: North-Holland) p 168
Borovik A A and Krasilinec V N 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** 1941
Bubelev V E and Grum-Grzhimailo A N 1990 *Opt. Spectrosc.* **69** 178
Buckman S J and Clark C W 1994 *Rev. Mod. Phys.* **66** 539
Cleff B and Mehlhorn W 1974 *J. Phys. B: At. Mol. Phys.* **7** 593
Fano U 1961 *Phys. Rev.* **124** 1866
Feldman P and Novick R 1967 *Phys. Rev.* **160** 143
Feuerstein B, Grum-Grzhimailo A N, Bartschat K and Mehlhorn W 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** 3727
Feuerstein B, Grum-Grzhimailo A N and Mehlhorn W 1998 *J. Phys. B: At. Mol. Opt. Phys.* **31** 593
Kavei G, Ottley T W, Pejčev V and Ross K J 1977 *J. Phys. B: At. Mol. Phys.* **14** 2923
Kaur S and Srivastava R 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** 2323
Kuchiev M Y and Sheinerman S A 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 2027
Matterstock B, Huster R, Paripas B, Grum-Grzhimailo A N and Mehlhorn W 1995 *J. Phys. B: At. Mol. Opt. Phys.* **28** 4301
Migdalek J and Kim Y-K 1998 *J. Phys. B: At. Mol. Opt. Phys.* **31** 1947
Ogurtsov G N 1983 *J. Phys. B: At. Mol. Phys.* **16** L745
Pejčev V and Ross K J 1977 *J. Phys. B: At. Mol. Phys.* **10** 2935
Read F H 1977 *J. Phys. B: At. Mol. Phys.* **10** L207
Rojas H L, Borovik A A and King G C 1995 *Proc. XIXth Int. Conf. on the Physics of Electronic and Atomic Collisions (Whistler, NY)* ed J B Mitchell *et al* (Amsterdam: North-Holland) p 463
Zatsarinny O I 1999 Private communication