The single ionization cross-section of Rb atoms by electron impact

2015 J. Phys.: Conf. Ser. 635 052004

(http://iopscience.iop.org/1742-6596/635/5/052004)

The single ionization cross-section of Rb atoms by electron impact

V. Roman* [1], **A. Kupliauskiene**† [2], **and A. Borovik***

*Department of Electron Processes, Institute of Electron Physics, Uzhgorod, 88017, Ukraine
†Institute of Theoretical Physics and Astronomy, Vilnius University, Vilnius, 01108, Lithuania

Synopsis The 5s+core single ionization cross-section of Rb atoms was calculated for the incident electron energies up to 600 eV by using the relativistic distorted-wave, Coulomb-Born and binary-encounter-dipole approximations. The accuracy of the data was analyzed by the comparison with experimental data. The best agreement was observed for the calculations performed in configuration interaction approximation.

The correct account for the contribution from indirect processes such as autoionization is very important problem of the theory of electron-impact ionization of atoms [1]. For instance, the single ionization of Rb atoms by electron impact was the subject of many theoretical studies (see e.g. [2] and references therein) but all of them failed to describe correctly the behavior of the experimental cross-section above the $4p^6$ excitation threshold. Meanwhile, there is a unique possibility to evaluate the accuracy of different theoretical techniques in accounting for indirect processes when along with the total ionization cross-section σ_{tot}, the autoionization cross-section σ_{aut} is also known experimentally [3].

In the present work we calculated the 5s+core single direct ionization cross-section of Rb atoms in relativistic distorted-wave (RDW), Coulomb-Born-Exchange (CBE) and binary-encounter-dipole (BED) approximations by using the FAC computer code [4]. In order to evaluate the role of correlation effects, the RDW and BED calculations were performed both in single configuration and configuration interaction (CI) approximations. In the case of CI calculations, the superposition of configurations $4p^6nl$ (n = 5, 6, 7, l = 0, 1, 2, 3), $4p^5nln'l'$ (nl = 5s, 6s, 5p, 4d, 5d, 4f, $n'l'$ = 5s, 6s, 5p, 6p, 4d, 5d, 4f, 5f, 5g) for the initial and $4p^6$, $4p^5nl$ (nl = 5s, 6s), $4p^4nln'l'$ (nl = 5s, 5p, $n'l'$ = 5s, 5p, 4d, 5d) for the final states was used to take into account the correlation effects. Figure 1 shows these data compared with the difference $\sigma_{tot}[5]$-$\sigma_{aut}[6]$ which represents the “true” 5s+core single direct ionization cross-section (see [3]).

As can be seen, significant discrepancies are observed in absolute values and energy behaviors of all calculated cross-sections around 10 eV and near the $4p^6$ ionization threshold. However, when compared with the “true” single direct ionization cross-

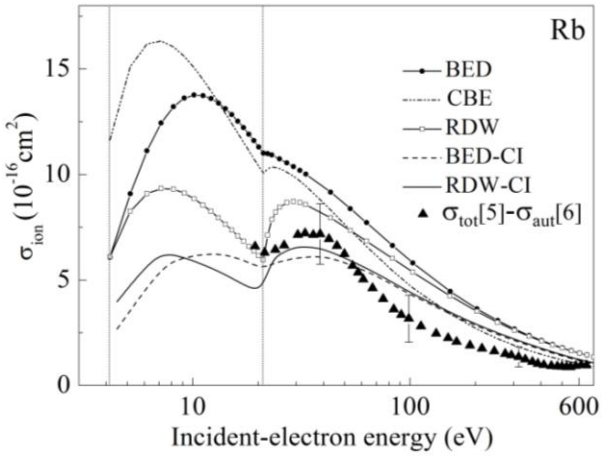

Figure 1. The single direct ionization cross sections of Rb atoms. Vertical dashed lines mark the 5s and $4p^6$ ionization thresholds at 4.18 and 20.71 eV [7], respectively.

section $\sigma_{tot}[5]$-$\sigma_{aut}[6]$ the RDW-CI and BED-CI data show the best agreement in the impact energy region just above the $4p^6$ ionization threshold. That points out the important role of correlation effects in electron impact ionization of inner shells in Rb atoms.

This research was funded by the National Academy of Sciences of Ukraine (project 0112У002079).

References

[1]D.L. Moores, K.J. Reed 1994 *Adv. At. Mol. Opt. Phys.* **34** 301
[2]M. Łukomski *et al* 2006 *Phys. Rev. A.* **74** 032708
[3]A. Borovik *et al* 2012 *J. Phys. B.* **45** 045204
[4]M. F. Gu 2008 *Can. J. Phys.* **86** 675
[5] J. Tate, P. Smith 1934 *Phys. Rev.* **46** 773
[6]A. Borovik *et al* 2013 *J. Phys. B.* **45** 215201
[7]J. E. Sansonetti 2006 *J. Phys. Chem. Ref. Data* **35** 301

[1] E-mail: viktoriyaroman11@gmail.com

[2] E-mail: alicija.kupliauskiene@tfai.vu.lt