Electron-impact excitation and ionization of K atom

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INTRODUCTION

Electron impact ionization cross-sections are widely used in applications such as modeling of plasma syntheses in tokamaks, modeling of radiation effects for both materials and medical research and aeronomy, as well as in basic research in astrophysics, atomic, molecular and plasma physics. Therefore, the study of ionization of atoms is very relevant today. This is confirmed by a large number of experimental and theoretical studies of the ionization process of atoms, in particular alkali metal atoms [1–4]. Previously, we studied the ionization cross sections for the rubidium atom [5]. Here we consider the capabilities of the most widely used theoretical approaches, relativistic Coulomb-Born (CB) distorted-wave (DW) and binary-encounter-dipole (BED), for the single electron impact ionization of the K atom in the impact energy range from the 4*s* threshold up to 700 eV using the standard software package Flexible Atomic Code [6].

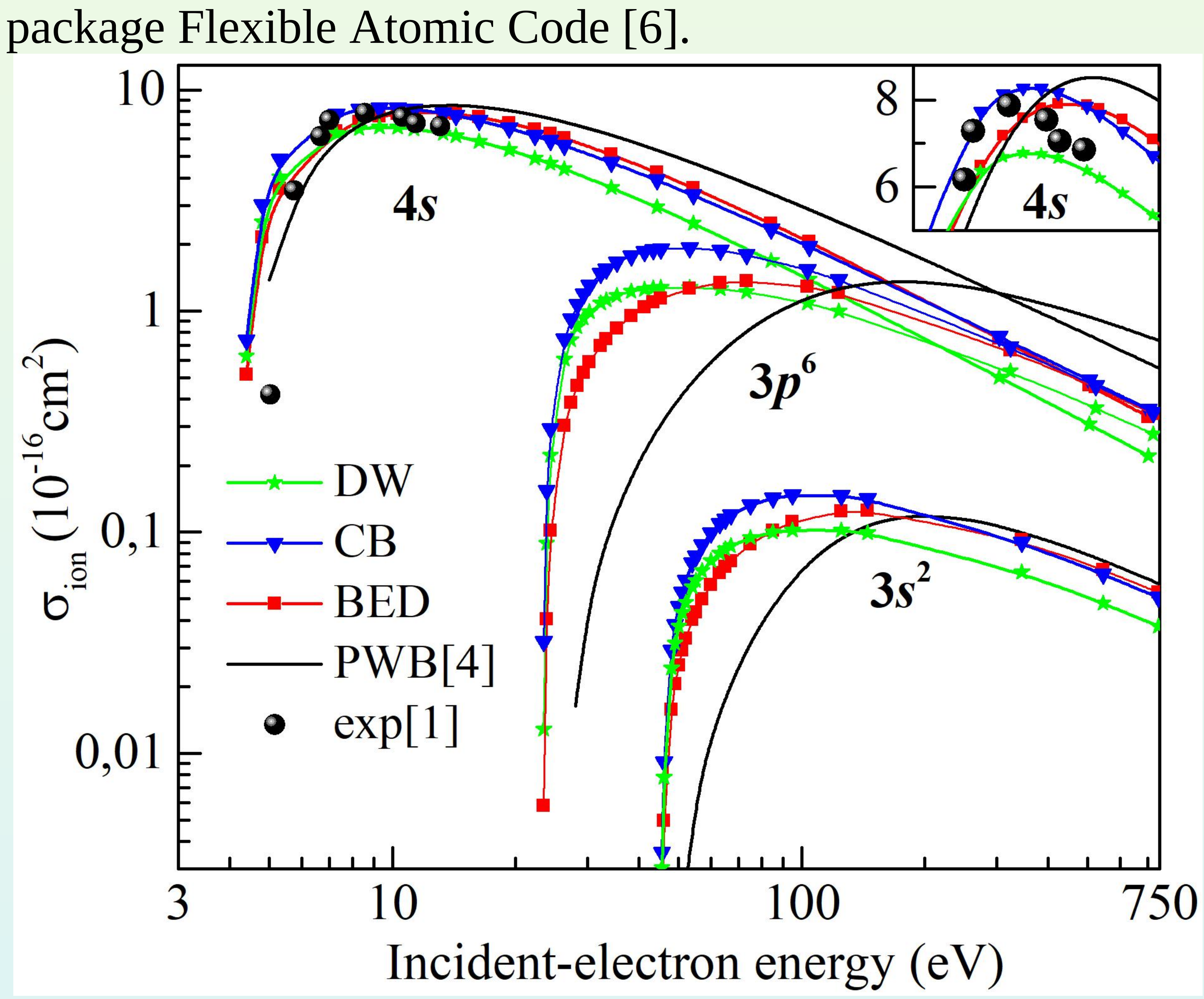

Figure 1. *The single ionization cross-sections of the 4s, $3p^6$, and $3s^2$ shells of the K atom.*

RESULTS and DISCUSSION

Figure 1 shows a comparison of the single ionization cross-sections of the 4*s*, $3p^6$, and $3s^2$ shells of the K atom calculated in the DW, BED, CB approximations with the data [4] obtained using the plane wave Born (PWB) approximation. Note that the experimental data are available only for the 4*s* shell and only below the excitation threshold of the $3p^6$ shell [1]. In fig. 1 these data [1] are normalized to the absolute values from [2] at 500 eV.

The comparison of the ionization cross-sections of the 4*s* shell shows that the absolute values of the BED data are the best match with the experiment, however the maximum of the cross-section is strongly shifted. As for the maxima position, the CB and DW data are in the best agreement with the experiment. The 4*s*-shell ionization cross-section obtained using PWB approximation [4] shows the largest discrepancy with experiment regarding the absolute values as well as maxima position.

As for the K atom $3p^6$ and $3s^2$ shells, their ionization cross-sections strongly differ between themselves. Unfortunately, it is impossible to experimentally obtain a cross-section of a specific electron shell. For this reason, we have now calculated the excitation cross sections of the K atom. This allowed us to isolate this indirect process from the full ionization cross section and obtain only the full cross section of the direct ionization of the potassium atom ($4s+3p^6+3s^2$). This will make it possible to estimate the correct description of both excitation and ionization of the deeper $3p^6$ and $3s^2$ shells. Figure 2 shows the excitation cross sections of the $3p^6$ and $3s^2$ shells of the K atom. The calculations were performed in the approximation of relativistic distorted waves within the framework of the Flexible Atomic Code software package [6].

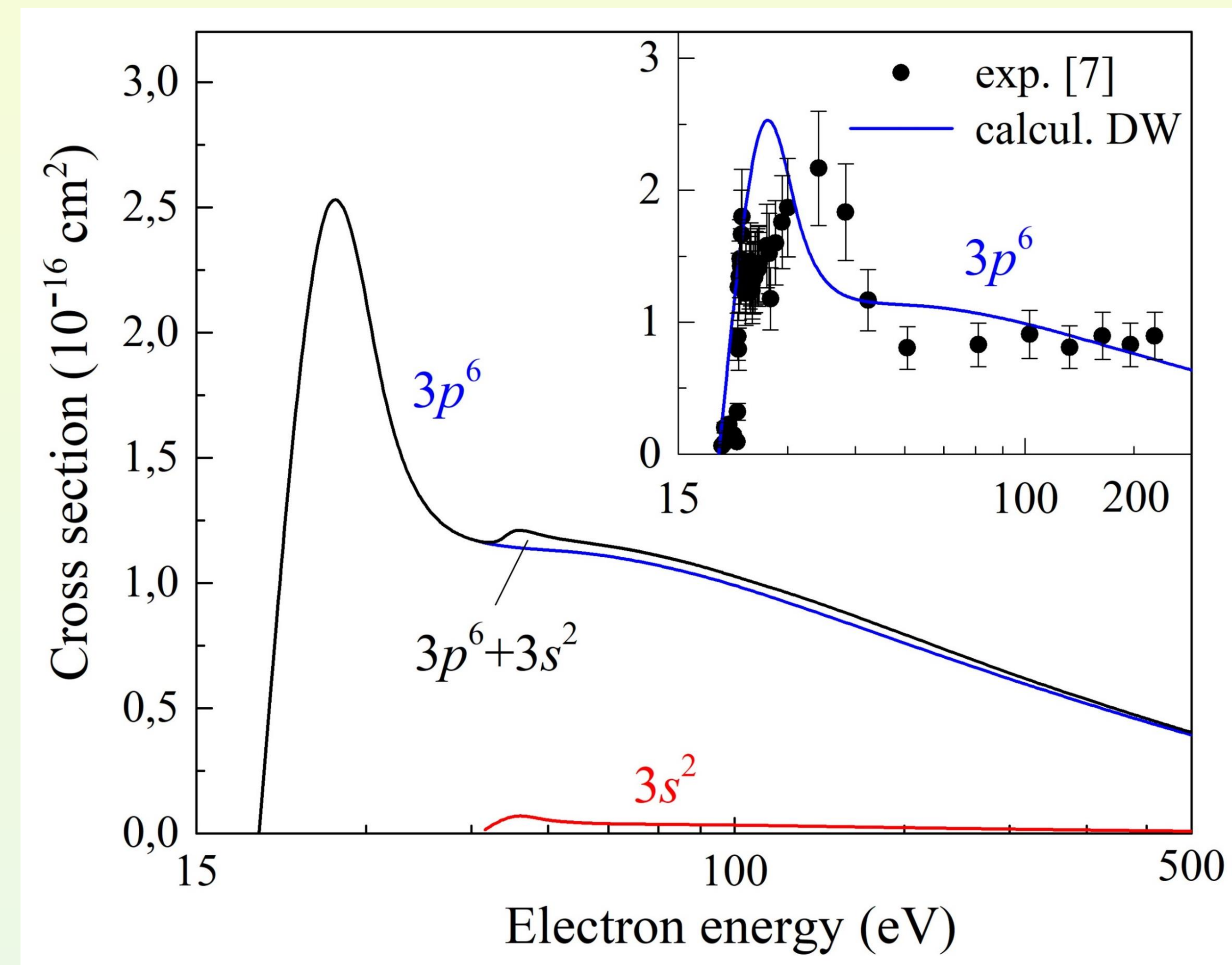

Figure 2. *Experimental excitation-autoionization [7] and calculated $3p^6+3s^2$ excitation cross sections of K atom.*

The excitation cross section of the $3p^6$ shell was obtained as the sum of the excitation cross sections of 96 autoionization states of the configurations $3p^5\,4s^2$, $3p^5\,3d4s$, $3p^5\,4s4p$, $3p^5\,4s5s$, $3p^5\,3d5s$, $3p^5\,4d4s$. Similarly, the 3*s*2 shell excitation cross section is the sum of 38 calculated excitation cross sections of autoionization states of configurations $3s\,4s^2$, 3*s* 4*s*4*p*, 3*s* 4*s*4*d*, 3*s* 4*s*5*s*, 3*s* 4*s*3*d*, 3*s* 5*s*5*p*, 3*s* 4*s*6*s*. A comparison with experimental data of the excitation cross section of the $3p^6$ shell [7] (see inset in Fig. 1) shows a satisfactory agreement with our calculations.

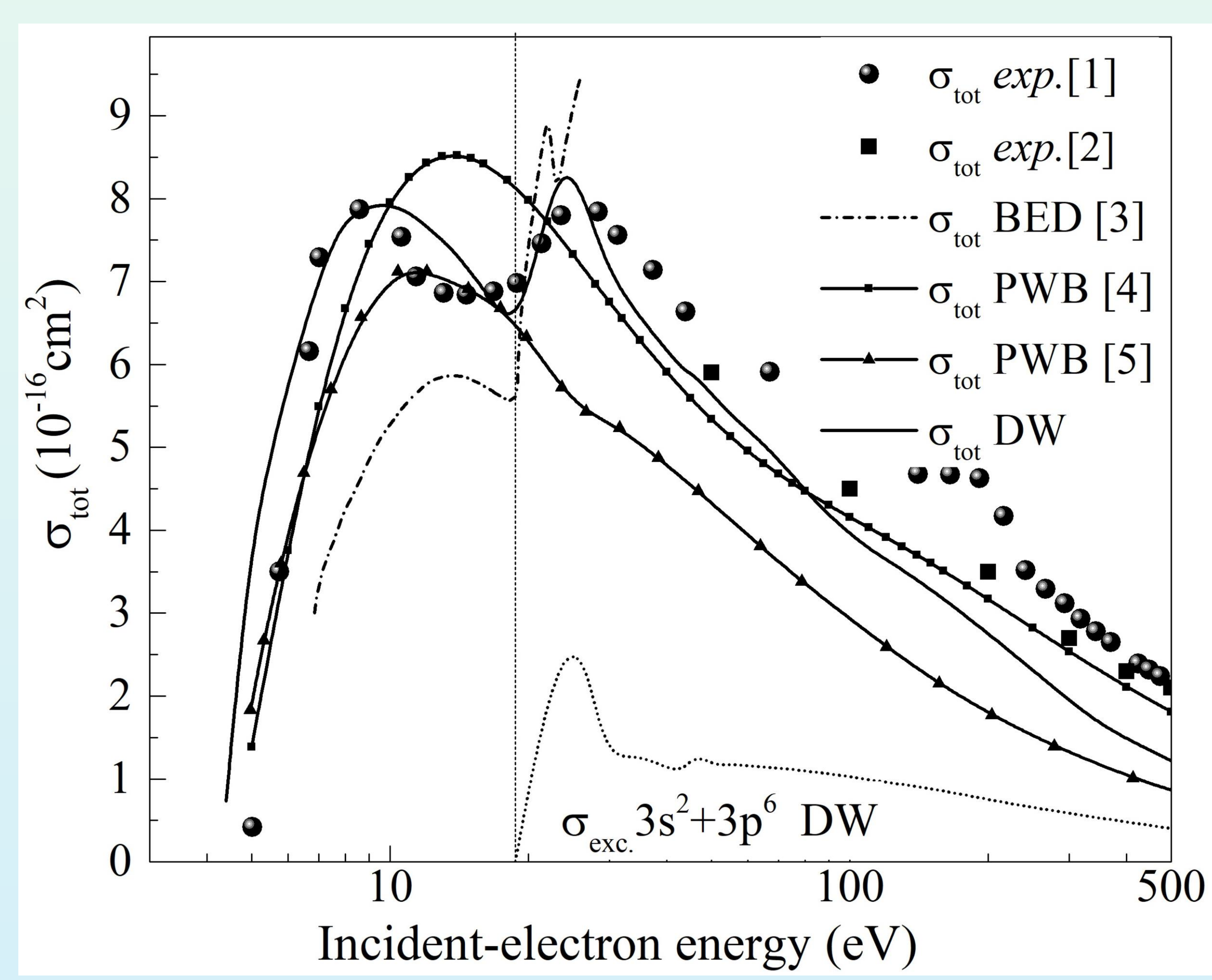

Figure 3. *The total ionization cross-sections of the K atom*

As the analysis shows (Fig.3), the total ionization and autoionization cross sections calculated by us, obtained in the DW approximation, best correspond to the experimental ionization cross section. Our study showed that the excitation of the $3s^2$ shell contributes 7% to the autoionization cross section and ≈1.5% to the total ionization cross section of the K atom. At the same time, it is shown that the excitation of the $3p^6$ shell is the main process of the autoionization of the K atom and contributes 29% to its full single ionization cross section.

References

[1] Tate J, Smith P 1934 *Phys. Rev.* **46** 773
[2] Mcfarland R *et al* 1965 *Phys. Rev.* **137** 1058
[3] Roy B, Rai D 1973 *Phys. Rev. A.* 8 849
[4] Bartlett P *et al* 2004 *Atomic Data and Nuclear Data Tables* **86** 235
[5] Roman V *et al* 2015 *J. Phys. B.* **48** 205204
[6] Gu M 2008 *Can. J. Phys.* **86** 675
[7] Borovik O, JTP 82, 18 (2012).