Energy threshold in multiple ionization by electron or positron impact

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Abstract. The energy threshold for the formation of highly charged ions is experimentally well-known and measured. For single ionization, it is the binding energy of the outermost electrons. For multiple ionization, the ionization begins at impact energies much larger than the theoretically expected ones. In this contribution we present a simple expression for the energy threshold for multiple ionization by electron or positron impact. It was obtained as the mean value of the energy transferred to each ionized electron by using Thompson classical approximation. Present results reproduce quite well the experimental thresholds. Moreover, the inclusion of these values in the theoretical multiple ionization cross sections allows describing rather well the experimental data for single up to sextuple ionization of rare gases.

1. Introduction

Electron impact ionization is a basic and active field within the atomic collisions. Most of the multiple ionization experimental values are from electron impact processes [1, 2]. Also in recent years the investigation on ionization by positron impact has received considerable attention (for example, the work of Laricchia and collaborators [3]). In both, electron and positron impact, multiple ionization cross sections depend smoothly on the impact energies in the intermediate to high energy range. But for low energies they fall down drastically, several orders of magnitude, when the energy gets close to certain value. These thresholds, or appearance energies, are clearly observed experimentally [4, 5]. For single ionization the threshold is the energy gap of the outermost sub-shell. However, for N-fold ionization the threshold is much larger than N times this energy. And the difference increases with N, *i.e.* the experimental threshold for quintuple ionization of Kr is around 200 eV $>> 5 \times E_{4p} = 71\ eV$.

In a recent theoretical work on multiple ionization by electron impact [2] not null cross sections were obtained for energies below the experimental threshold. The aim of this contribution is to correct this failure by proposing a value for the appearance energy as the mean energy transferred to the emitted electrons, enough to jump to the continuum and to leave the target with a certain mean kinetic energy.

2. Theoretical model

We calculate the mean energy transfer by resorting to a classical model by Thompson [6]. Briefly, if we consider the scattering problem of two charged particles (charges Z_1 and Z_2, velocities v_1 and v_2, masses m_1 and m_2), the transferred energy is

$$\Delta E = \frac{1}{2}m_2(v_2^2 - v_{2f}^2) = \frac{1}{2}m_2(v_{1f}^2 - v_1^2). \tag{1}$$
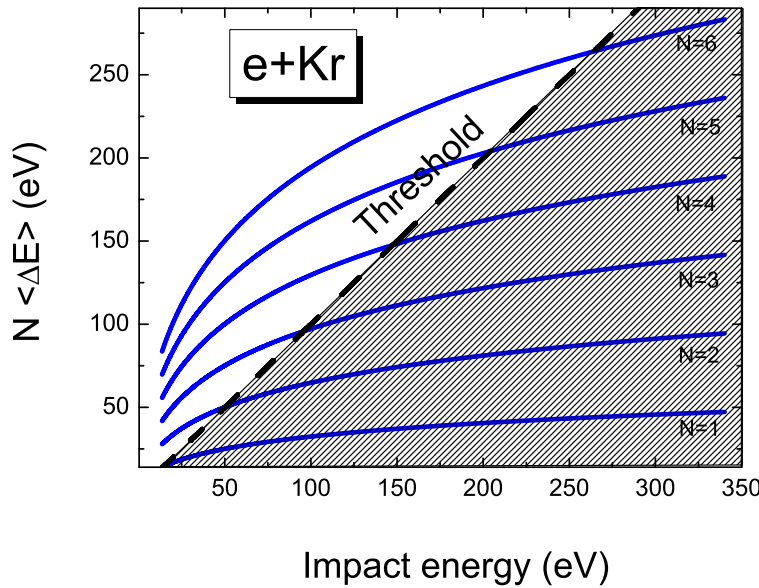
Figure 1. Mean energy transferred in multiple ionization by electron impact, as function of the impact energy (solid-lines). The dashed-line is the impact energy, and the shaded region indicates $E > N \times < \Delta E_{nl} >$.

Considering the momentum and energy conservation and assuming $v_1 << v_2$, the differential cross section in the transferred energy is

$$\frac{d\sigma}{d(\Delta E)} = \frac{2\pi \ (Z_1 Z_2)^2}{m_1 v_2^2 \ (\Delta E)^2},$$ (2)

and the total cross section to emit an electron of the nl sub-shell is

$$\sigma_{nl} = \int_{I_{nl}}^{E_{max}} \frac{d\sigma}{d(\Delta E)} \ d(\Delta E) = \frac{2\pi \ (Z_1 Z_2)^2}{m_1 v_2^2} \ (\frac{1}{I_{nl}} - \frac{1}{E_{max}}),$$ (3)

with I_{nl} being the ionization energy of the nl sub-shell, $E_{max} = \frac{4 \ m_1 m_2}{(m_1 + m_2)^2} E$ being the maximum energy transferred, and E the impact kinetic energy of particle 2 [6]. In the case of electron-electron interaction, replacing charges and masses in (3), the ionization cross section in Thompson approximation is expressed as

$$\sigma_{nl} = \frac{\pi}{E \ I_{nl}} \left(1 - \frac{I_{nl}}{E}\right).$$ (4)

Following the same procedure we can calculate the stopping cross section as

$$S_{nl} = \int_{I_{nl}}^{E_{max}} \Delta E \ \frac{d\sigma}{d(\Delta E)} \ d(\Delta E) = \frac{\pi}{E} \ Ln(E/I_{nl}).$$ (5)

This logarithmic dependence with the impact energy is similar to Bethe stopping, valid in the high energy region. Then we calculate the mean energy transferred $< \Delta E_{nl} >$ to ionize an electron initially in the nl sub-shell as

$$< \Delta E_{nl} >= \frac{S_{nl}}{\sigma_{nl}} = \frac{E \ I_{nl} \ Ln(E/I_{nl})}{(E - I_{nl})}.$$ (6)
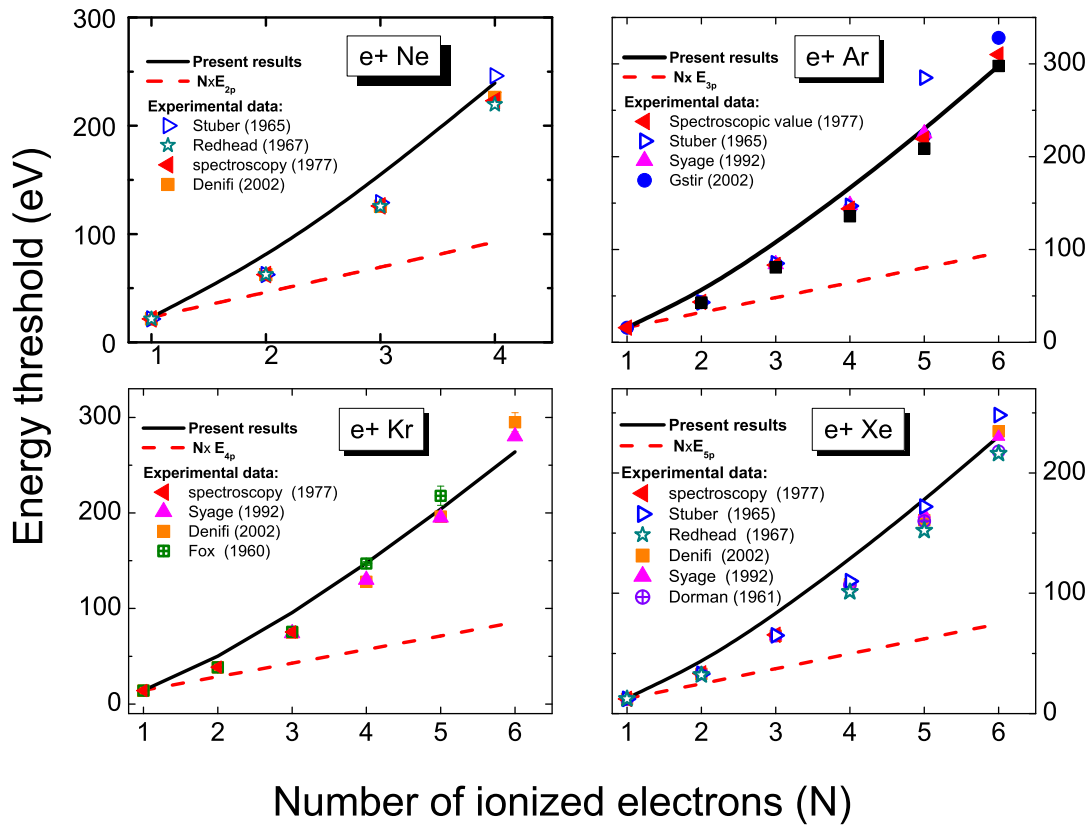
Figure 2. [colour online] Energy threshold for multiple ionization by electron or positron impact. Curves: black-solid, present results; red-dashed line, the binding energy of the outer sub-shell per the number of ionized electrons. Symbols: experimental data, details in the insets and references in [4, 5]; red left-triangles, spectroscopy data [7]

In this model we propose that the minimum impact energy for N-fold ionization of the nl sub-shell is $N \times \; < \Delta E_{nl} >$. In figure 1 we display the mean energy transferred given by (6) as function of the impact energy E, for ionization of the $4p$ sub-shell of Kr. We also include in this figure the straight line corresponding to the electron impact energy. The energy region where the multiple ionization is allowed is indicated as a shaded area.

3. Results and discussions

We compare the present results for Ne, Ar, Kr and Xe with the experimentally known energy thresholds [4, 5]. In figure 2 we show $N \times < \Delta E_{np} >$ for the outer np electrons of each target. We also include the value $N \times E_{np}$ to emphasize the difference between them. The improvement in the description of the experimental energy thresholds is clear. The advantage is more evident for quadruple to sextuple ionization.

Finally in figure 3 we display the triple ionization cross sections of Kr by electron impact. The solid black curve was obtained using the present energy minimum, while the red-dashed curve is our previous calculation considering $N \times E_{np}$ as energy threshold. A detailed explanation of the calculation of the multiple ionization cross sections and of the experimental data included
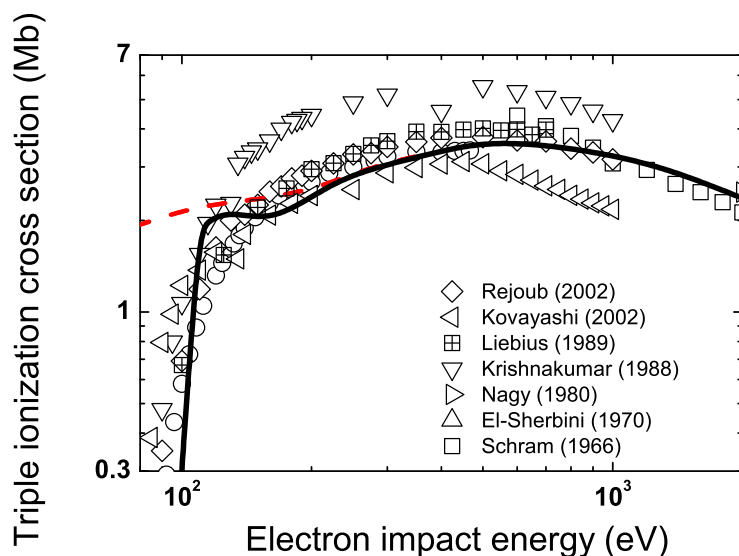
Figure 3. [colour online] Triple ionization of Kr by electron impact. Curves: black-solid line, CDW-EIS results including present expression for the energy threshold; red-dashed line, similar values considering just the binding energy of each shell [2]. Symbols, compilation of experimental data in [2]

in this figure is in [2].

4. Conclusions
We calculate the energy threshold for multiple ionization by electron impact, by using Thompson classical model for the ionization cross section as function of the transfer energy. The results show very good agreement with the experimental thresholds obtained using different technics. We also show that this approximation improves previous multiple ionization cross sections in the region near the threshold.

Acknowledgments

References
[1] Shevelko V and Tawara H 1998, *Atomic Multielectron processes* (Springer-Verlag, Berlin Heidelberg)
[2] Montanari C C and Miraglia J E 2014, *J. Phys. B: At. Mol. Opt. Phys.* **47**, 105203
[3] Laricchia G, Cooke D A, Kover A, Brawley S J 2013 *Experimental Aspects of IonizationStudies by Positron and Positronium Impact* (Cambridge University Press), Vol **56**, pp.116-136
[4] Gstir B, Denifl S, Hanel G, Rümmele M, Fiegele T, Cicman P, M Stano, Matejcik S, Scheier P, Becker K, Stamatovic A and Märk T D 2002, *J. Phys. B: At. Mol. Opt. Phys.* **35** 2993-3007
[5] Denifl S, Gstir B, Hanel G, Feketeova L, Matejcik S, Becker K, Stamatovic A, Scheier P, and Märk T D 2002, *J. Phys. B: At. Mol. Opt. Phys.* **35** 4685-4694
[6] McDowell M R C and Coleman J P 1970, *Introduction to the theory of ion-atom collisions*, (North-Holland Pub. Co.), chapter 3
[7] Rosenstock H M, Draxl K, Steiner B W and Herron J T 1977 *Energetics of gaseous ions, J. Phys. Chem. Ref. Data* 6 (suppl. 1)