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Relativistic calculations of *K*-, *L*- and *M*-shell X-ray production cross-sections by electron impact for Ne, Ar, Kr, Xe, Rn and Uuo

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ABSTRACT

In this work, we derive X-ray production cross-sections from electron-impact ionization cross-sections for Ne, Ar, Kr, Xe, Rn, and Uuo, calculated in the modified relativistic binary-encounter-Bethe model, and using as the only input parameter the binding energies obtained in the Dirac-Fock approach. Radiative and radiationless transition probabilities necessary to compute the inter- and intra-shell atomic yields were calculated in the same approach. Shell electron-impact ionization cross-sections and X-ray production cross-sections are compared with the corresponding cross-sections retrieved from the National Institute of Standards and Technology Reference Database and available experimental data.

1. Introduction

Electron-impact ionization cross-sections (EIICS) and X-ray production cross-sections (XRPCS) are fundamental quantities that describe the interaction of electrons with mater and subsequent production of X-rays. This knowledge is important in several fundamental and applied fields.

Electron-impact ionization and excitation have been actively studied by many research groups since the 1920s. Most of the work produced was based on classical collision theory, leading to the development of several first principle theories (see, for example [1], for a brief review of the subject). Seminal work in the field of electron-atom collisions was made by Bethe [2,3] who derived the correct form of the ionization cross section for high-energy collisions using the plane-wave Born approximation (PWBA). Since then, several empirical and semi-empirical models have been proposed to describe electron-impact ionization of atoms and molecules [4–9] and several reviews of the relevant literature were published (see, for instance, [10]).

Existing models can be divided into three types: (a) those based on classical mechanics, which provide simple expressions at the cost of accuracy; (b) those based on quantum mechanics, more accurate than their classical counterparts but at the cost of higher complexity; (c) the semi-empirical ones, which are often also based on the classical formulations.

The classical models for electron-impact ionization are suitable for describing collisions in which the momentum transfer is large. With the advance of quantum mechanical computational methods, some very sophisticated *ab initio*

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theories became available, as the convergent close coupling (CCC) [11], the *R*-matrix [12,13], and the exterior complex scaling [14] approaches. Nevertheless, most calculations are very time-consuming, limiting the domain of applicability of the models employed [15,16]. Empirical and semi-empirical models can be very simple to use and provide a good estimate of the cross sections for a wide range of elements and subshells. However, as experimental cross sections are scarce for some elements and subshells, it is challenging to benchmark the robustness of such models for the entire range of elements, shells and energies. More recently, several analytical expressions have been developed to overcome these constraints, some of them empirical [17,18] and others derived from first principles [19–24]. The latter are still widely used in all the above mentioned fields of physics, even when the large and steady increment in computational power seems to consistently privilege numerical computations.

Precise experimental data are needed to provide a benchmark against which to test current theories. See, for instance, [10,25,26], and references therein regarding available experimental data for EIICS and XRPCS in rare gases.

In this work, we present calculations of XRPCS by electron-impact, in the energy range between 10 eV and 100 MeV for Ne, Ar, Kr, Xe, Rn, and Uuo ($Z=118$). The EIICS were obtained using the modified relativistic binary-encounter-Bethe (MRBEB) model derived by our group [1]. This model has been applied in the study of specific isonuclear series [27] and its robustness and consistency successfully tested against the configuration-averaged distorted-wave (CADW) [28], Distorted Wave Born Approximation (DWBA) [29,30], the widely used Lotz formula [9,31], and available experimental results.

The multi-configuration Dirac–Fock (MCDF) computer code MCDFGME, developed by Desclaux and Indelicato [32,33] was used to obtain the subshell binding energies and transition probabilities for the *K*-, *L*-, and *M*-subshells. The latter were used to compute the inter- and intra-shell vacancy transfer yields published in [34].

Total EIICS calculated in the MRBEB model are compared with the PWBA calculations of Barlett and Stelbovics [35], and the experimental data of A.A. Sorokin et al. [36,37]. Inner-shell cross-sections are compared with the corresponding cross-sections from the NIST Standard Reference Database (NIST164) [38], obtained from a model developed by Bote and Salvat that corrects the low-energy behaviour of PWBA cross-sections with a scaling factor obtained from semi-relativistic DWBA calculations [39–41]. XRPCS are also compared with the NIST164 database cross-sections and the compilation of experimental values from [25] for the *K*-shell and other few experimental data for the *L*-shell.

2. Calculation of cross-sections

2.1. Electron-impact ionization cross-sections

The MRBEB model is a modification of the RBEB model [20], the relativistic counterpart of the binary-encounter-Bethe (BEB) model, that combines the Mott cross section with the high incident electron's kinetic energy behavior of the Bethe cross section within the relativistic framework. Both BEB and RBEB models use different scaling factors, depending on the subshell to be ionized, in order to reproduce the experimental data [1,42]. Although this type of scaling has been inserted in several theories such as the PWBA, its success remains to be explained, even though it is a practical way to account for the electron exchange, distortion, and polarization effects that are absent in the first-order PWBA.

Instead of using different energy scaling factors, the MRBEB model adopts a single term $X_{S_j}(Z_{\mathrm{eff}})$, where S_j designates the subshell ($S=K$; $S=L$ with $j=1,2,3$; $S=M$ with $j=1,\ldots,5$; etc) to be ionized. This term accounts for the screening of the nuclear charge by the inner atomic electrons, and can be approximated by a quadratic function of the effective nuclear charge Z_{eff},

$$X_{S_j}(Z_{\mathrm{eff}}) = a\frac{Z^2_{\mathrm{eff},S_j}}{2n^2_S} + b\frac{Z^2_{\mathrm{eff},S'_i}}{2n^2_{S'}}, \tag{1}$$

where n_S and $n_{S'}$ are, respectively, the principal quantum numbers of the orbital to be ionized (corresponding to the S_j subshell) and of the orbital immediately above in the energy scale (corresponding to the S'_i subshell). Subshell Z_{eff} values were provided by the MCDFGME code, although the atomic screening constants can also be obtained in the literature (see for example [43,44]). Alternatively, the Z_{eff} can be determined from the well-known approximation that considers it to be given by the difference between the atomic number and the number of inner electrons up to the relevant subshell. The constants $a=0.3$ and $b=0.7$ were determined from experimental analysis across the whole Z spectra [1]. Since there is no occupied shell above the valence one, the scaling term for the highest occupied shell is simply obtained by setting $a=1$ and $b=0$ in Eq. (1).

According to the MRBEB model, the EIICS is given by

$$\sigma^I_{S_j} = \frac{4\pi a_0^2\alpha^4 N_{S_j}}{(\beta_t^2+\chi_{S_j}\beta^2_{b,S_j})2b_{S_j}}\left\{\frac{1}{2}\left[\ln\left(\frac{\beta_t^2}{1-\beta_t^2}\right)-\beta_t^2 - \ln(2b_{S_j})\right]\left(1-\frac{b^2_{S_j}}{t^2}\right)+1-\frac{b_{S_j}}{t} - \frac{\ln(t/b_{S_j})}{1+t/b_{S_j}}\frac{1+2t}{(1+t/2)^2}+\frac{b^2_{S_j}}{(1+t/2)^2}\frac{t/b_{S_j}-1}{2}\right\}, \tag{2}$$

where the reduced parameters are defined as

$$t\equiv T/mc^2 \quad b_{S_j}\equiv B_{S_j}/mc^2$$
$$\beta_t^2\equiv 1-\frac{1}{(1+t)^2} \quad \beta^2_{b,S_j}\equiv 1-\frac{1}{(1+b_{S_j})^2}$$
$$\chi_{S_j}\equiv X_{S_j}(2R/B_{S_j}), \tag{3}$$

with T representing the kinetic energy of the impacting electron, and B_{S_j} is the binding energy of the electron in the subshell S_j. The dimensions of the cross-section are set by the constant $4\pi a_0^2\alpha^2 N_{S_j}$, where a_0 is the first Bohr radius, α is the fine structure constant, and N_{S_j} is the occupation number of the subshell S_j to be ionized. The constants m and R in the definitions of the reduced