Mg 2p ionization by electron impact

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The ionization of Mg 2p by electron impact has been studied at about 400 and 1000 eV incident energy and small momentum transfer via $(e, 2e)$ experiments. Two kinematical conditions have been chosen in order to study the coincidence angular distribution in the case where either only the direct 2p ionization contributes or the decay of the 2p core hole plays a role, too. The results have been compared with distorted-wave Born approximation calculations.

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Electron impact ionization of atoms and molecules is one of the basic processes in nature. Ionizing collisions are relevant to a wealth of scientific and technological areas such as gas discharges, cold plasmas, lasers, and the chemistry of the upper atmosphere. Moreover, their theoretical understanding involves the modeling of the few-body Coulomb interaction. As such electron impact ionization has attracted much experimental and theoretical interest.

The best way to characterize the dynamics of an electron impact ionization is to detect the scattered and ejected electrons in coincidence. The quantity measured in these $(e, 2e)$ experiments is the triple-differential cross section (TDCS) $d^3\sigma/d\Omega_a d\Omega_b dE_a$ —i.e., a cross-section differential in the solid angles of the ejected and the scattered electrons, labeled by a and b , respectively, and in the energy of one of them. The energy of the other is determined by energy conservation, $E_a + E_b = E_0 - V_i$, where E_0 is the energy of the incident electron and V_i is the ionization energy of the target.

In the case of atomic hydrogen and helium the improvement of the experimental techniques [1–3] and recent developments of theoretical approaches [4–8] have led to a detailed understanding of the process. Investigation of inner-shell ionization still presents significant challenges to both theory and experiments. Accurate measurements are difficult due to the low values of the cross section and the long accumulation times, even with the multidetection setups. This limits the region of the kinematical parameters that can be investigated. On the theoretical side the influence of the nucleus on the incident and scattered electrons and the interaction between the target electrons and the scattered electron as well as the final-state interaction between ejected and scattered electrons have to be taken into account. Then the relaxation of the inner hole via the nonradiative Auger decay results in a final state with three electrons in the continuum. The Auger electron can exchange energy and angular momentum with the other continuum electrons, and when the kinetic energies of at least two of these electrons are close, then interference effects may occur. Finally, the energy balance of an $(e, 2e)$ inner-shell process does not guarantee that

the detected electron pair originates from the inner-shell ionization. Double ionization of the valence shell may also occur, and the two electrons belonging to such a process are also detected; i.e., an $(e, (3-1)e)$ measurement is done [9]. The third undetected electron carries the “missing” energy. Thus also the interference between the single- and double-ionization processes may contribute to the observed TDCS.

Magnesium is a good candidate for the study of the inner-shell ionization. The binding energies of the $2p_{3/2,1/2}$ orbitals are 57.54 and 57.81 eV, respectively. This allows study of the inner-shell ionization without loss of orders of magnitude in the count rate. van Boeyen *et al.* [10,11] studied the ionization of Mg 2s, 2p, and 3s between 400 and 3000 eV incident energy in an asymmetric kinematics where the ejected electrons are detected off-plane in two opposite truncated hemispherical analyzers, equipped with eight detectors arranged around a 45° cone. The energy of the ejected electrons and the angle of the scattered electrons were chosen in order to have a large momentum transfer ($|\vec{K}| = |\vec{K}_0 - \vec{K}_a| \geq 1.8$ a.u.) and the direction of $\vec{K}$ pointing toward the two analyzers. In their first paper [10] van Boeyen *et al.* exploited the symmetry or the lack of symmetry of the TDCS about $\vec{K}$ to test the approximations used to describe the ionization process. In the second [11] paper they investigated the contribution of two-step processes, involving one ionizing collision and a second elastic collision with the core, to the measured TDCS. They found that also in the two-step ionization the information on the momentum distribution of the orbital was kept. Recently Bolognesi *et al.* [12] studied the ionization of Mg in asymmetric kinematics at about 1000 eV incident energy and $K < 2$ a.u. The most interesting observation was that in the studied kinematics the characteristics of the initial-state wave function determined the main features of the TDCS.

In this work the ionization of Mg 2p has been studied at about 400 and 1000 eV incident energy in asymmetric kinematics. The angle of the fast electron has been chosen to have always $K \approx 1$ a.u. Moreover, in one measurement the

energy of the ejected electrons has been set equal to the one of the unresolved $L_{2,3}$ -MM Auger electrons to investigate interference and exchange effects between ejected and Auger electrons.

A crossed-beam apparatus has been used to measure the TDCS of Mg. Since the apparatus has been recently described in detail elsewhere [12], only information relevant to the present measurements will be reported here. The vacuum chamber contains an electron gun, two twin 180° hemispherical electrostatic analyzers rotatable independently in the scattering plane, and a resistively heated, anti-inductively wound oven to produce the atomic beam of Mg. The scattered electrons ($E_a=400$ or 1000 eV) were detected at a fixed angle θ_a , while the angle θ_b of the ejected electrons ($E_b=20$ or 35 eV) was varied from 50° to 130° . The pass energies of the two analyzers were chosen to have energy resolutions of $\Delta E_a=3.1$ and 1.6 eV at $E_a=400$ or 1000 eV, respectively, and $\Delta E_b=1.6$ and 0.8 eV at $E_b=20$ or 35 eV, respectively. These resolutions do not allow to resolve the two $\text{Mg}^+ 2p$ spin orbit components; thus, both states contribute to the measured TDCS. The typical incident current in the measurements was about $5 \mu\text{A}$.

The experiments have been compared with calculations [8] performed in the distorted wave Born approximation, (DWBA). The TDCS for ionizing an electron from the (n, l) shell of a target atom is given by

$$\frac{d^3\sigma}{d\Omega_a d\Omega_b dE_a} \propto \frac{k_a k_b}{k_0} \sum_m [|f_{nlm}|^2 + |g_{nlm}|^2 - \text{Re}(f_{nlm}^* g_{nlm})]. \quad (1)$$

Here the sum over m is a sum over the magnetic substates of the (nl) shell. $f_{nlm}(\vec{k}_a, \vec{k}_b)$ and $g_{nlm}(\vec{k}_a, \vec{k}_b)$ are the direct and exchange amplitudes for the ionization process, respectively. These amplitudes are given by

$$f_{nlm} = \langle \chi^-(\vec{k}_a, \vec{r}_a) \chi^-(\vec{k}_b, \vec{r}_b) | 1/r_{ab} | \chi^+(\vec{k}_0, \vec{r}_a) \psi_{nlm}(\vec{r}_b) \rangle, \quad (2a)$$

$$g_{nlm} = \langle \chi^-(\vec{k}_a, \vec{r}_b) \chi^-(\vec{k}_b, \vec{r}_a) | 1/r_{ab} | \chi^+(\vec{k}_0, \vec{r}_a) \psi_{nlm}(\vec{r}_b) \rangle. \quad (2b)$$

In Eq. (2a) and (2b), ψ_{nlm} is the target bound-state wave function and χ^+ and χ^- are distorted waves of the electrons in the initial and final states, with outgoing (+) and ingoing (−) scattered wave boundary conditions. The target wave function $\psi_{nlm}(\vec{r}) = R_{nl}(r) Y_{lm}(\vec{r}/r)$ is a product of the radial orbital [13] and a spherical function. The incoming distorted wave χ^+ was calculated in the static exchange potential of the neutral target. The outgoing distorted wave χ^- of the fast scattered electron was calculated both in the static-exchange potential of the neutral atom and in the one of the singly charged final ion. The outgoing distorted wave χ^- of the slow ejected electron has been calculated in the static-exchange potential of the final ion state. Local exchange potentials of Furness-McCarthy type [14] were used to simplify the static exchange calculation. The final-state distorted waves are orthogonalized to the target orbital. To understand better the physics of the process also a first Born (FB) calculation, where the incident and scattered electrons are described by

FIG. 1. (Color online) TDCS of Mg $2p$ at $E_a=400$ eV, $E_b=20$ eV, and $\theta_a=10.5^\circ$ (a) and 5.5° (b). The solid and dashed lines represent the DWBA and FB predictions, respectively. The bold arrows indicate the $\vec{K}$ and $\vec{K}_a$ directions.

plane waves, has been performed. This means that the multiple-scattering effects involving elastic scattering of the incident electron by the atom prior ionization, or elastic scattering of the faster outgoing electron by the ion after the ionization, are neglected. The final-state interaction between the electrons has been included in the calculations using the Gamow factor N_{ee} , which gives an approximate treatment of the post-collision interaction [15,16].

The TDCS measured at $E_a=400$ eV, $E_b=20$ eV, and $\theta_a=10.5^\circ$ and 5.5° are shown in Figs. 1(a) and 1(b), respectively, while the ones measured at $E_a=1000$ eV, $E_b=20$ and 35 eV, and $\theta_a=7^\circ$ and 3.5° are shown in Figs. 2 and 3. The data at $E_a=1000$ eV, $E_b=20$, and $\theta_a=7^\circ$ were already presented in Bolognesi *et al.* [12]. There was a small input file error in the DWBA calculations presented earlier [12]. It makes a very slight difference in the calculation and in no way alters the conclusions of the earlier paper. However, a comparison between experiment and the corrected calculations is reported here for sake of completeness.

The TDCSs in asymmetric kinematics are characterized [17] by the presence of two lobes. The first one, nearly in the direction of $\vec{K}$, is associated with a binary collision of the incident electron, and it is named the “binary peak.” The second peak, near the opposite direction, is known as the “recoil peak,” since it is commonly associated with a back-scattering of the ejected electron from the atomic nucleus.

FIG. 2. (Color online) TDCS of Mg $2p$ at $E_a=1000$ eV, $E_b=20$ eV, and $\theta_a=7^\circ$. The solid and dashed lines represent the DWBA and FB predictions, respectively. The bold arrows indicate the $\vec{K}$ and $\vec{k}_a$ directions.

The relative intensity of the two lobes, their width, and their position with respect to $\pm\vec{K}$ are the observables that provide the information on the dynamics of the process.

The main features observed in the experimental TDCS in Figs. 1 and 2 are the dominance of the recoil lobe and the split of the binary lobe. These observations are in complete agreement with previous results on inner-shell ionization—for example, in the case of Ar $2p$ [18–21]. The split binary lobe is due to the p character of the ionized orbital, whose momentum distribution is characterized by a node at $q=0$, where $|\vec{q}|=|\vec{k}_a+\vec{k}_b-\vec{k}_0|$ is the momentum of the ejected electron before the collision in the hypothesis of a binary event. As discussed in a recent paper by Kampp *et al.* [8] in the plane-wave Born approximation (PWBA) the direct scattering amplitude f is proportional to the initial-state wave function in momentum space. Thus the TDCS follows the behavior of the $2p$ momentum distribution which rises from $q=0$ to a local maximum and then decreases monotonically as q increases. The kinematical condition which allows one to

FIG. 3. (Color online) TDCS of Mg $2p$ at $E_a=1000$ eV, $E_b=35$ eV, and $\theta_a=3.5^\circ$. The solid and dashed lines represent the DWBA and FB predictions, respectively, while the dash-dotted line is a representation of the experimental data with an Auger angular distribution (see text). The bold arrows indicate the $\vec{K}$ and $\vec{k}_a$ directions.

achieve $q=0$ is called the bound Bethe ridge kinematics. In such a condition in PWBA a zero in the TDCS is expected. This zero becomes a minimum of TDCS when distortion effects, needed, for example, to describe a low-energy ejected electron, are taken into account [8]. Another effect of the distortions is a shift with respect to the $\vec{K}$ direction toward larger θ_b . If the kinematics does not comply with the bound Bethe ridge condition, a minimum in the TDCS may still exist. This is exactly the situation in the present experiment where at $\theta_b=60^\circ$ and 70° in Figs. 1(a) and 2, respectively, the minimum q value ($q \approx 0.1$ a.u.) is reached. The minimum at $\theta_b=45^\circ$ in the experimental TDCS of Fig. 1(b) is not completely justified by an initial-state effect because $q=0.45$ a.u. Indeed both theories predict only a shallow minimum in this kinematics. The large increase of the recoil lobe, previously studied, for example, in Ar both experimentally and theoretically [20], has been attributed to two factors. The first one is a double-scattering process in which the incident electron backscatters elastically off the nucleus and then ionizes the target, and the second one is the strong final-state interaction between the slow ejected electron and the nucleus. Both effects are included implicitly in the DWBA through the distorted waves of the electrons, and the calculations satisfactorily describe the experimental results.

The FB calculation predicts a TDCS very similar in shape to the one of the DWBA. However DWBA, consistently with the experiment, predicts a slightly asymmetric TDCS with respect to the $\vec{K}$ direction and a small shift toward larger θ_b ($\approx 10^\circ$). This effect, already observed in Ne and Ar [21], stems from the strong static potential of “heavy” atoms, which is particularly important in inner-shell ionization since the ionization process occurs close to the nucleus, where the static potential is at its strongest [21]. The overall satisfactory agreement with the FB indicates that the observed TDCS are essentially due to the direct ionization of the $2p$ orbital and the contribution of the double ionization of valence shell is negligible. This is not unexpected for collision processes at small K where single ionization is known to have its largest cross section. The good agreement between the DWBA and FB predictions clearly shows that double-scattering events for the fast electrons are not very important in these kinematics. A comparison of the calculations with and without the N_{ee} factor shows that this factor changes slightly the relative intensities of the binary and recoil peaks, but not the general shape of the TDCS. This is justified by the large relative velocity of the scattered and ejected electrons, which limits their mutual interaction.

The TDCSs have not been measured on an absolute scale; thus, the calculations have been rescaled independently to the experiment at the maximum of the recoil lobe in each figure. However, in the measurements at $E_a=400$ eV (Fig. 1) where only θ_a is changed, the experimental relative intensity of the two TDCSs at $\theta_b=110^\circ$ is 0.57 ± 0.1 . The DWBA and FB calculations predict ratios of 0.49 and 0.47, respectively, in good agreement with the experiment. As for the absolute values, however, it has to be noted that in the investigated conditions the predicted values by the two models differ of about 30%.

The results at $E_a=1000$ eV, $E_b=35$ eV, and $\theta_a=3.5^\circ$

(Fig. 3) display a different shape compared to the TDCSs measured in the other kinematical conditions. An almost isotropic angular distribution is observed. The absence of a minimum in the binary peak may be explained by the minimum value of q (0.95 a.u.) achieved. However the theoretical predictions of two lobes of almost equal intensities in the case of the DWBA or with a small prevalence of the binary peak in the FB calculation are far from the experiment. At this E_b both the directly ejected and the Auger electrons produced in the decay of the $2p$ hole contribute to the electron spectrum, with the latter largely dominating the spectrum. Indeed the ratio between the unresolved $L_{2,3}-M_1M_1$ Auger peak and the underlying continuum is about 16. Thus coincidences between the fast-scattered and Auger electrons (e, e' Auger) are likely to dominate the observed TDCS. Already in the 1970s [22] it had been observed that the angular distribution of Auger electrons displays an anisotropy due to the alignment of the intermediate ionic state. In the case of the $L_{2,3}-M_1M_1$ Auger electrons for the decay of the $Mg^+ 2p$ ion only the $L_3-M_1M_1$ one can contribute to the asymmetry in the angular distribution, because the $Mg^+ 2p_{1/2}$ inner state is not aligned. In the two-step approximation the (e, e' Auger) coincidence angular distribution can be expressed as [23]

$$\frac{d^3\sigma}{d\Omega_a d\Omega_b dE_a}(\theta_a, \theta_b) \propto [1 + \beta P_2 \cos(\theta_b - \theta_K)], \quad (3)$$

where β is the asymmetry parameter of the angular distribution of the Auger electrons, which is related to the alignment parameter $A_{20}(2p^5 3s^2 {}^2P_{3/2})$ of the inner-shell hole [$\beta(L_3-M_1M_1) = 2A_{20}(2p^5 3s^2 {}^2P_{3/2})$] [24]], and θ_K is the direction of $\vec{K}$. The fit of Eq. (3) to the experiment using β and a scaling factor as free parameters is represented by the dash-dotted line in Fig. 3. The best fit gives $\beta = 0.09 \pm 0.05$, which is consistent with the value of 0.16 ± 0.01 obtained by Kammerling *et al.* [25] at $h\nu = 80$ eV, a photon energy close to the energy loss of the present experiment. The value of A_{20}

obtained agrees within the respective uncertainties with the one obtained in a noncoincidence experiment of DuBois *et al.* [26]. These results prove that in this kinematics the TDCS is dominated by the indirect process. This alters the angular distribution with respect the one expected in the direct ionization. However, no peculiar interference features due to the indistinguishability of the two electrons are observed. This is also consistent with the observation that the electron energy spectrum is largely dominated by the Auger electrons.

In summary, the $Mg 2p$ ionization has been studied at two incident and ejected electron energies and low momentum transfer. Two different kinematics have been investigated. In the first one, where the direct ionization of the $2p$ orbital has been studied, first-order DWBA models give a satisfactory representation of the experiment. In the second kinematics where the selected kinetic energy makes the electrons ejected in the ionization process indistinguishable from the Auger electrons emitted in the decay of the inner hole, the TDCS appears to be completely determined by the decay process. However, at variance with the recent results in Ar [27], where a large anisotropy in the TDCS has been observed and attributed to interference effects between $2p$ ionization and the direct and indirect—i.e., via Auger decay—double ionization, here only a small anisotropy, which is due to the alignment of the intermediate ionic state, has been observed. In this latter kinematics the DWBA is unable to describe the experimental TDCS. These results together with previous experiments in Ar [19,20,27] and Xe [28] show that the inclusion of the decay channel in the current DWBA models for inner-shell ionization by electron impact is a highly desirable improvement of the model and should extend its successful application to electron impact ionization of atoms.

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