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Electron-impact ionization of the *K* shell of silver and gold in coplanar asymmetric geometry

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Triple differential cross sections are presented for the electron-impact ionization of silver and gold in coplanar asymmetric geometry at an impact energy of 500 keV. The problem is treated in a completely relativistic manner, using Dirac distorted waves in both the incident and final channels and the full photon propagator. Good agreement with experiment is obtained.

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In recent years significant progress has been made in understanding the physics of electron-impact ionization at nonrelativistic energies. The development of coincidence techniques has allowed for experiments almost at the limit of what is quantum mechanically knowable, and much has been learned about the dynamics and kinematics of the ionization processes. The theoretical description of the $(e,2e)$ processes has been developed and improved recently. For an overview of the different approaches used we refer to reviews covering this field [1–3]. The inner-shell ionization of heavier noble gases at a few keV impact energy shows in particular many similarities to the collision systems under investigation here. Excellent agreement has been obtained there between the experimental triple differential cross sections (TDCS's) and those calculated in the distorted-wave Born approximation [4]. At relativistic impact energies absolute experiments within an accuracy of 15% by Nakel and collaborators for the K-shell ionization of heavy-metal targets in coplanar symmetric and asymmetric geometry have existed for some time [5–9]. The theoretical studies of this process reported so far employ modifications of the relativistic first Born approximation with either plane waves for all electrons [10], or semirelativistic Coulomb waves for at least one unbound electron [8,11–13]. In asymmetric geometry all these calculations overestimate the experimental cross sections; the discrepancies increase with the atomic number of the target. Walters *et al.* [8] showed that in coplanar symmetric geometry it is important to include spin-flip contributions and argued that the distorting effect of the nucleus and the electron cloud in the incident as well as in the final channels cannot be neglected for inner-shell ionization in all geometries. Pinzola, Moores, and Griffin developed a relativistic distorted-wave formalism [14] and applied it to calculate singly differential electron-impact ionization cross sections. In this contribution we report first results for TDCS's using a fully relativistic distorted-wave Born approximation.

The TDCS is given by (in atomic units)

$$\frac{d\sigma_{(e,2e)}}{d\Omega_1 d\Omega_2 dE_2}=\frac{(2\pi)^2}{c^6} N_i \frac{k_1 k_2}{k_0} E_0 E_1 E_2 \, \tfrac{1}{4} \sum_{\text{all spins}} |S^{\text{dir}} - S^{\text{ex}}|^2, \quad (1)$$

where 0, 1, and 2 indicate the incoming and the two outgoing electrons, respectively, N_i is the number of electrons in the shell considered, and

$$S^{\text{dir}}=i\int d^4x \int d^4y J^{\mu}_{10}(x) D_{\mu\nu}(x-y) J^{\nu}_{2b}(y). \quad (2)$$

Here $D_{\mu\nu}(x-y)$ is the complete QED photon propagator in the Coulomb gauge and $J^{\mu}_{10}(x)$ and $J^{\nu}_{2b}(y)$ are transition matrix elements of the Dirac four currents

$[J_{ij}^{\mu}(x)=\bar{\psi}_i(x)\gamma^{\mu}\psi_j(x)]$ generated in the static field of the atom. The exchange matrix elements $S^{\rm ex}$ are obtained by interchanging all quantum numbers of the outgoing electrons.

To evaluate $S^{\rm dir}$ and $S^{\rm ex}$ the time integrals are solved analytically. The spatial parts of the scattering waves are expanded in partial waves. The radial wave functions are computed numerically using the code of Salvat and Mayol [15], which is based on the power series expansion of Bühring [16]. The effective atomic potentials going into this calculation are obtained from a self-consistent relativistic Kohn-Sham calculation using the local-density approximation [17]. The photon propagator is also expanded in multipoles. This allows for the angular integrals to be done using angular-momentum algebra, whereas the radial integrals are computed numerically [18–20]. In a first series of calculation, we have used the potential of a neutral atom to compute all the distorted waves, and have approximated the K-shell wave function by a relativistic hydrogenic $1s$ state. We checked that the overlap between the bound state and the partial waves is negligible. Twenty-two partial waves were used for the incident electron and 28 for the fast scattered electron, and the multipole sum of the interaction was terminated after the sixth term. By the sum rules arising from the angular integrals, the number of partial waves contributing to the slow outgoing electron is fixed to the number of multipoles of the expansion of the interaction. We took care that this was sufficient to obtain satisfactory convergence. As a further cross-check we calculated the corresponding plane-wave approximation using the same number of partial waves and multipole terms and compared it with analytic results. This we felt was a useful test, since the plane-wave case is often slower to converge. Secondly we checked the nonrelativistic limit by comparing our data with the calculation of Zhang *et al.* [4] for the ionization of neon $(1s^2)$ at 2.7 keV. For a detailed description of the theory, the test procedures, and the convergence behavior we refer to our subsequent paper [21]. Nevertheless, due to the four spinor structure of the wave functions the above set of parameters still requires the evaluation of about 40 000 radial integrals and literally millions of vector coupling coefficients.

In Fig. 1, we present results for the K-shell ionization of gold in coplanar asymmetric geometry at an impact energy of 500 keV. The fast outgoing electron possesses an energy of 319 keV and the slow one 100 keV. The detection angle for the fast electron is fixed at $-15°$; the TDCS is plotted against the ejection angle of the slow electron relative to the beam axis. We compare our results (solid line) with the experimental data from Bonfert, Graf, and Nakel [7] (the error bars show the statistical but not the systematical uncertainty) and with theoretical calculations from Das and Konar [11] (dotted line), Jakubassa-Amundsen [12] (dashed-dotted lines), and Walters *et al.* [8] (dashed line). Das and Konar use a semirelativistic Sommerfeld-Maue Coulomb wave function for the slow outgoing electron, Jakubassa-Amundsen uses nonrelativistic Coulomb functions multiplied by a free Dirac spinor for both outgoing electrons (dashed-dotted), while Walters *et al.* use a Darwin-Coulomb wave for the slow electron, a plane wave for the fast electron, and include spin-flip contributions (dashed). It is obvious that the distortion of all unbound wave functions by the atomic potential in the present calculation leads to a significant decrease of the TDCS and to a shift of the binary peak, resulting in a good agreement with the absolute experimental data available [7]. It should be noted here that the DWBA calculation is not normalized to the experimental data.

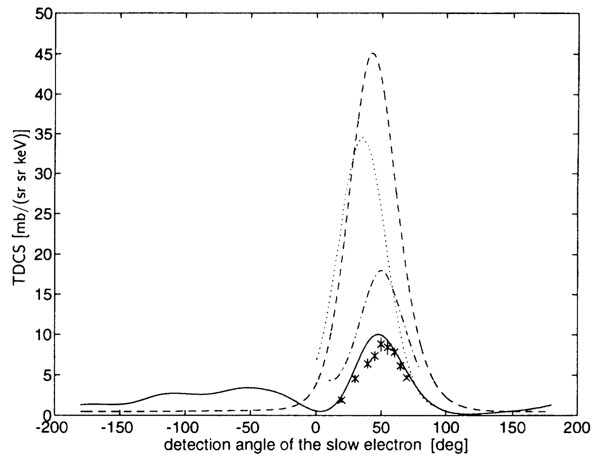

FIG. 1. Triple differential cross section for K-shell ionization of gold by electron impact plotted against the angle of the slow outgoing electron. Impact energy, 500 keV; energy of the fast electron, 319 keV; energy of the slow electron, 100 keV; the detection angle of the fast electron is fixed at $-15°$. ×, experimental data, Bonfert, Graf, and Nakel [7]; · · ·, plane-wave Born, Das and Konar [11], no spin-flip contributions; — — —, plane-wave Born, Walters *et al.* [8], including spin flip; —·—·— Coulomb-Born Jakubassa-Amundsen [12], no spin-flip; ——, present results.

In Fig. 2 a TDCS for a silver target in the same geometry is shown. Here the angle of the fast outgoing electron is fixed at $-7°$ and the energy values are $E_1=375$ keV, $E_2=100$

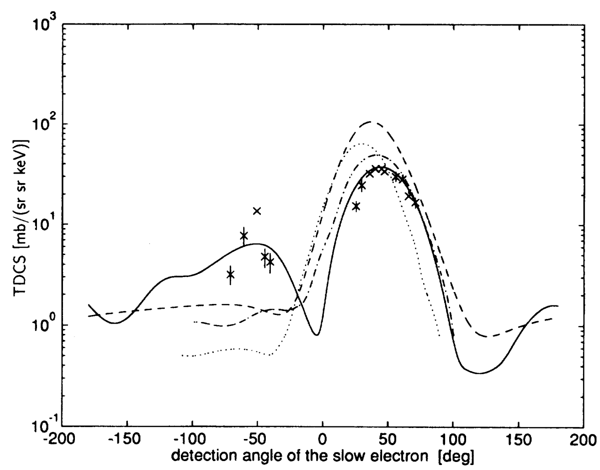

FIG. 2. Triple differential cross section for K-shell ionization of silver by electron impact plotted against the angle of the slow outgoing electron. Impact energy, 500 keV; energy of the fast electron, 375 keV; energy of the slow electron, 100 keV; the detection angle of the fast electron is fixed at $-7°$. ×, experimental data, Bonfert, Graf, and Nakel [7]; · · ·, plane-wave Born, Das and Konar [11], no spin-flip contributions; — — —, plane-wave Born, Walters *et al.* [8], including spin flip; —·—·—, Coulomb-Born Jakubassa-Amundsen [12], no spin-flip; ——, present results.

keV for the same impact energy. Again in our calculation the binary peak is described well in both shape and magnitude. An additional peak in the recoil region is visible where we find some discrepancies in detail between the experimental data and the results of our calculation. In particular, the cross sections at $\theta_2 = -50°$ differ significantly. This discrepancy is under investigation in close collaboration with Nakel and co-workers [7]. Other calculations available, which do not include distortion effects, have not even reproduced the order of magnitude of the TDCS in the recoil region relative to the binary peak.

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