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Low Energy Inner Valence Ionization Of The Rare Gases

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Abstract. Recent measurements are presented of the triple differential cross section for electron impact ionization of the inner valence shells of argon and krypton at low to intermediate energies, and both coplanar symmetric and asymmetric geometries. Comparison is made with some of the latest available theoretical calculations performed in the distorted wave Born approximation formalism.

INTRODUCTION

In recent years, measurements of the triple differential cross section (TDCS) for low energy electron impact ionization in coplanar symmetric or energy-sharing geometry have provided a considerable challenge to modern scattering theories. The majority of these measurements were performed on hydrogen and helium targets [1], although a few measurements exist for heavier atoms [2]. Very recently, the first low impact energy experiments on an argon target in the coplanar asymmetric geometry have been performed [3,4], for both 3s and 3p ionization, as well as new measurements [5] for 3s ionization in the coplanar symmetric geometry. The coplanar symmetric and asymmetric geometries are illustrated schematically in Figure 1. In Refs. [3] and [4], comparison of the coplanar asymmetric TDCS with two different distorted wave Born approximation (DWBA) calculations [6,7] showed very poor agreement, particularly for the case of 3s ionization. The level of disagreement was rather surprising, since for incident energies greater than about 100 eV, the DWBA had been shown to exhibit quite good agreement with experiment for ionization of the rare gases. No theoretical calculations were available for comparison at the time the data for 3s ionization in the coplanar symmetric geometry were published, but these kinematics are expected to offer an even more stringent test of the theory.

In this paper, we review the current status and level of agreement between the latest theoretical and experimental results for argon. The new DWBA calculations shown here explore the importance of exchange in determining the form of the cross section,

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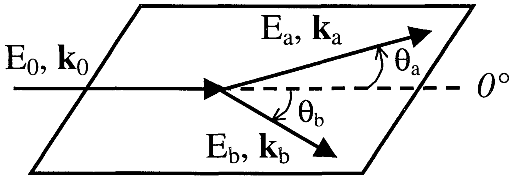

FIGURE 1. Diagram of the coplanar kinematics. The incident electron has energy and momentum E_0, $\mathbf{k}_0$. The scattered electron is detected at a scattering angle θ_a with energy E_a, while the ejected electron is detected with energy E_b at angle θ_b. θ_a and θ_b are measured from 0°, as shown. In the asymmetric measurements, θ_a is fixed while θ_b is varied. In the symmetric measurements both θ_a and θ_b are varied such that $\theta_a = \theta_b = \theta$.

and include results for coplanar symmetric argon 3s ionization. Details of the theory and the different approaches used to incorporate exchange may be found in Ref. [8]. We also present new measurements for the inner valence (4s) ionization of krypton, and contrast the form of the TDCS for this target with that obtained for 3s ionization in argon.

EXPERIMENTAL DETAILS

The electron coincidence spectrometer is shown schematically in overview in Figure 2. A detailed discussion of the apparatus may be found in Ref. [3]. Two identical hemispherical electron energy analysers, fitted with channel electron multipliers for electron detection, are mounted on concentric independent turntables. The analysers are mounted coplanar with the fixed electron gun; the incident electron beam crosses a target gas beam at right angles. Conventional coincidence timing electronics are employed. In the coplanar asymmetric measurements, the binary peak is measured by fixing the scattered electron energy analyzer at -15° with respect to the incident beam, and rotating the ejected electron energy analyzer through the desired angular range on the opposite side of the scattering plane. The recoil peak is measured by moving the scattered electron energy analyzer to +15° and again moving the ejected electron energy analyzer through the accessible angular range. The counting time at each ejected electron angle is normalized to a preset scattered electron count. As the measurements are not absolute, the binary-to-recoil ratio is determined in a separate measurement, as detailed in Ref. [3]. In the coplanar symmetric measurements, the two analyzers are rotated at equal angles on either side of the incident electron beam. Equal counting times are employed at each angle, and the incident current and gas pressure are carefully monitored to ensure no variation.

RESULTS AND DISCUSSION

Selected experimental and theoretical results for argon 3s and 3p ionization in the asymmetric geometry are presented in Figure 3. The incident energy is 113.5 eV and

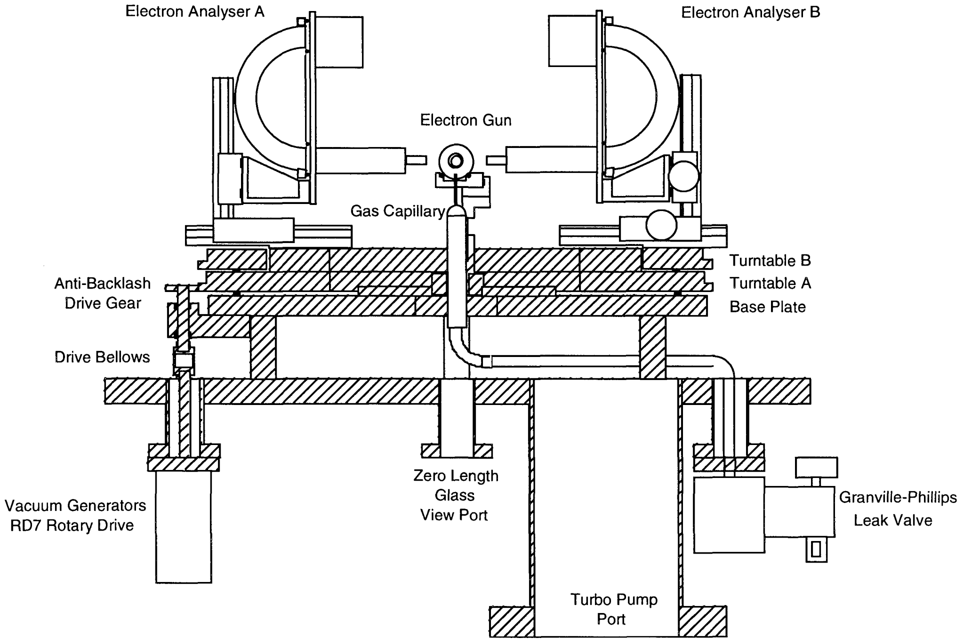

FIGURE 2. Schematic diagram of the electron coincidence spectrometer.

the ejected electron energies are 2 and 5 eV. The scattered electron energies are adjusted to meet the energy balance, with binding energies of 29.3 eV (3s) and 15.8 eV (3p). The scattering angle is 15°. The solid curve is the DWBA with no exchange, while the dashed line is the DWBA with the Furness-McCarthy [9] approximation to the static exchange potential (DWBA-FM), with the triplet potential used for the incident and faster final state electrons and a combination of triplet and singlet potentials used for the slower ejected electron. The experimental results have been normalized to the peak value in the binary region in the latter calculation. It is apparent that the treatment of exchange is very important for 3s ionization, particularly at 2 eV, where only the DWBA-FM gives even qualitatively the right shape. Overall, the agreement between theory and experiment is considerably better for 3p ionization than for 3s ionization. In the former case, both theories give a good description of the shape of the binary peak, and of the recoil-to-binary peak ratio. The major discrepancy is in the theoretical versus experimental position of the recoil peak. This difference cannot be attributed to post collision interaction (not fully accounted for in either theory) which would tend to move both binary and recoil peaks towards 180°. In the case of 3s ionization, there are still significant differences between theory and experiment in both the binary and, more dramatically, the recoil region. As the maximum of the recoil peak in the measured data appears to lie at a smaller angle than is experimentally accessible, it is not possible to compare the experimental and

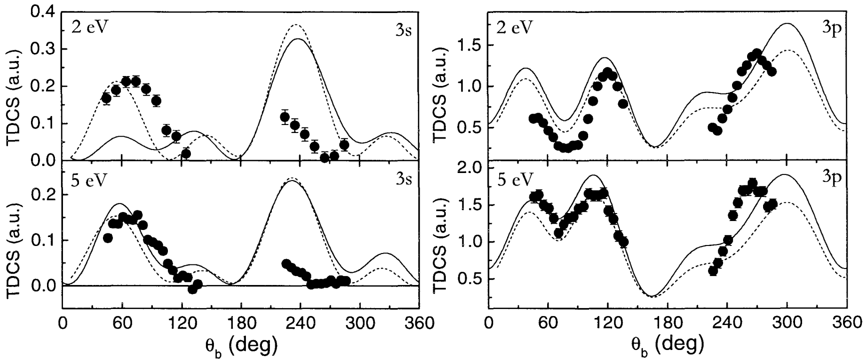

FIGURE 3. Triple differential cross section for argon 3s and 3p ionization in the coplanar asymmetric geometry. The incident energy is 113.5 eV, and the scattering angle is 15°. The ejected energy is shown on each graph, as is the orbital being ionized. The points are the experimental data. The solid line is a DWBA calculation without exchange, while the dashed line is a DWBA calculation with the Furness-McCarthy [9] exchange potential (see text). The experimental results have been normalized to the latter calculation in the binary region.

theoretical recoil-to-binary peak ratio, which normally provides a good test of the quality of the theory.

Figure 4 shows the results for argon 3s and krypton 4s ionization in the coplanar symmetric geometry. The solid line and dotted line are the DWBA and DWBA-FM calculations respectively. The dash-dot line is a DWBA calculation (labelled DWBA-1) we have performed using the McCarthy code [7]. The argon experimental results have been normalized to the DWBA-FM calculation at 40° for the case of 50, 20 and 10 eV outgoing energy. For the 4 eV case, the data have been normalized so as to give the same peak height as the DWBA-FM at backward angles. The krypton data have been normalized to the DWBA-1 at the forward peak. The DWBA-FM exhibits quite good agreement with the argon experimental data at 50 eV and 20 eV outgoing energy, even though the effect of PCI is underestimated at forward angles. At the lower outgoing energies, the DWBA (no exchange) appears to be in better shape agreement with the experimental data, although proper inclusion of PCI at these energies can be expected to change the form of the cross section substantially. The structure at forward angles in the TDCS has been attributed to a single electron-electron binary collision, with the structure at backward angles arising from a double binary collision in which the incident electron is first back-scattered from the nucleus and then undergoes a single binary collision with a bound electron [10]. The results show the evolution of the backward peak as the outgoing energy decreases, until at 4 eV the single binary peak has disappeared altogether and the double scattering peak has become the dominant structure. One interesting feature of the argon data at the higher energies is the forward position of the binary peak, which lies at a much smaller angle than 45°, where one would expect the peak to be located in an impulsive collision. In contrast, the krypton data at 85 eV, 50 eV and 20 eV outgoing energy

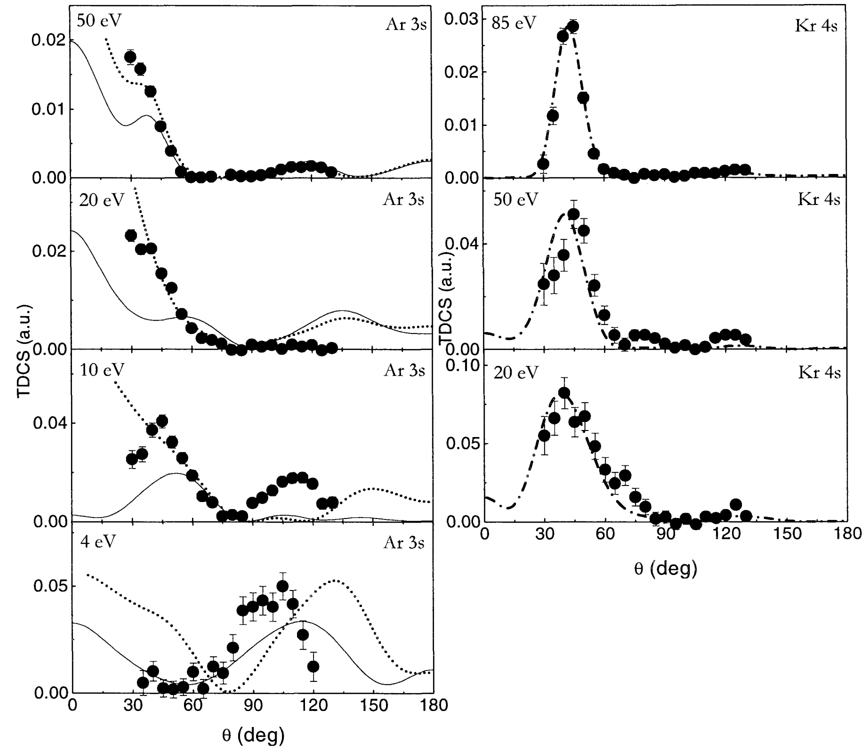

FIGURE 4. Triple differential cross section for argon 3s and krypton 4s ionization in the coplanar symmetric geometry. The outgoing electron energy is shown on each graph, as is the orbital being ionized. The points are the experimental data. The solid line is a DWBA calculation without exchange, the dotted line is the DWBA-FM calculation with the Furness-McCarthy [9] exchange potential and the dash-dot line is the DWBA-1 calculation using the code of McCarthy (see text). The experimental results have been normalized to the calculations as detailed in the text.

show a binary peak positioned near 45°. The DWBA-1 calculation is in very good agreement with the krypton experimental data, and has quite a different shape to the DWBA-FM calculation for argon at the same energies. The origin of the different behaviour of the TDCS for these two targets is not known.

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