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Electron double differential cross sections for ionization of O_2 under fast C^{6+} ion impact and interference oscillation

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Abstract
The absolute double differential cross sections (DDCS) have been obtained for electron emission from oxygen molecules under the impact of bare carbon ions. The DDCS values are measured between an energy range of a few eV to 600 eV and over an angular range of 30–150°. These are then compared with the continuum distorted wave-eikonal initial state (CDW-EIS) calculations. The DDCS values for O_2 are divided by that of atomic oxygen (calculated theoretically) to look for any oscillatory behaviour arising from Young-type interference. In addition, the DDCS ratios are further divided by a fitted straight line to extract any primary interference oscillation. Although a negative result has been obtained, these observations are in qualitative agreement with the prediction of the CDW-EIS model used.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Double differential cross section (DDCS) studies of low-energy electrons emitted in the ionization of medium-Z atoms and molecules by different projectiles have been reported in a few cases [1]. Also, it is well known, both theoretically [2, 3] and experimentally [4–6], that di-atomic molecules, in particular H_2, can act as natural double slits for electrons to interfere. But such studies are relatively scarce for multi-electron systems, except for some experimental work [7, 8] based on N_2 and O_2 and theoretical calculations [9] on N_2 ionization by fast proton impact. In this work, we have measured the absolute DDCS for electron emission in the ionization of oxygen molecules under the impact of 51 MeV bare carbon ions, to look for such effects.

Briefly, the experimental setup consists of a high-vacuum chamber equipped with a motorized turntable and a hemispherical electrostatic analyser for the measurement of the angular and energy distributions of ejected electrons. The scattering chamber was flooded with molecular oxygen as the target gas at an approximate pressure of 0.15 mTorr. For each angle, the number of electrons at different energies that were ejected in that direction was detected for a specified amount of incident projectile charge collected on a Faraday cup. The energy dependence of the DDCS was investigated for nine different emission angles between 30° and 150°. The error due to statistical fluctuation was 10–15% throughout the experiments. The uncertainty in the gas pressure was about 6–7%. Overall, the maximum possible error in the DDCS values is about 22%.

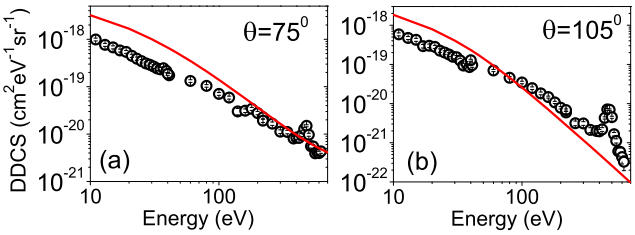

Figure 1. Absolute electron DDCS at two different emission angles of the secondary electrons. The solid line in each plot corresponds to the theoretical calculations using the continuum distorted wave-eikonal initial state (CDW-EIS) model.

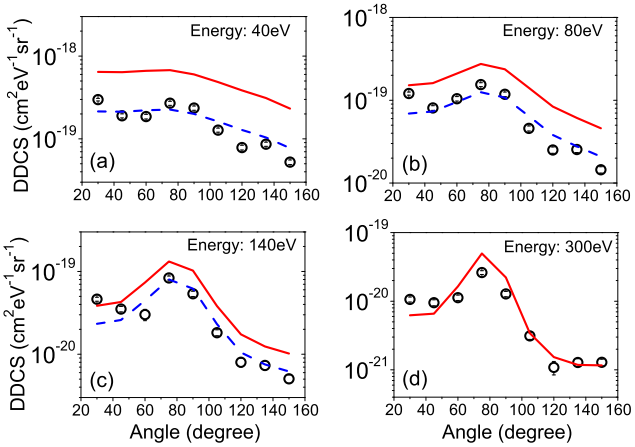

Figure 2. Absolute electron DDCS at different emission energies of the secondary electrons. The solid line in each plot corresponds to the theoretical calculations using the CDW-EIS model. The dashed lines in the plots are shown to display the qualitative agreement between theory and experiment. The 'scale-down' factors in (a), (b) and (c) are 3.0, 2.2 and 1.65, respectively.

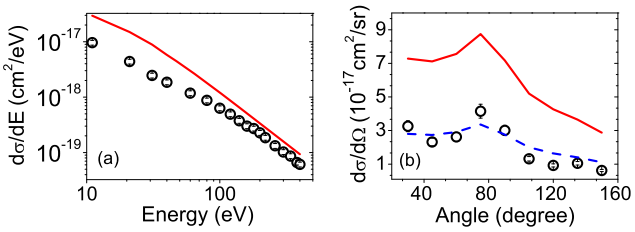

Figure 3. Absolute electron SDCS as a function of emission energies (a) and angles (b) of the secondary electrons. The solid line in each plot corresponds to theoretical calculations using the CDW-EIS model. The dashed line in (b) corresponds to theoretical values 'scaled down' by a factor of 2.6 to display the qualitative agreement between theory and experiment.

Table 1. $\frac{d\sigma}{dE}$ at different energies.

Energy (eV)	$\frac{d\sigma}{dE}$ (Mb eV^{-1})
11	9.622
21	4.391
31	2.461
40	1.860
60	1.183
80	0.875
100	0.632
120	0.493
140	0.375
160	0.301
180	0.272
200	0.227
220	0.185
260	0.132
300	0.102
340	0.086
380	0.066
400	0.061

2. Energy and angular distributions for DDCS

2.1. DDCS at fixed angles

The DDCS of the secondary electrons, as shown in figure 1 decrease with increasing electron emission energies. The enhancement in DDCS values at very low energies (∼10 eV) can be attributed to the soft collision processes, dominant in that particular region. The peak observed around 480 eV corresponds to the K-LL Auger transition for oxygen. Considering the complex nature of the target involved, the theoretical calculations based on the CDW-EIS model (for details, see [9]) reproduce only qualitatively the behaviour of the experimental DDCS spectrum. As far as quantitative agreement is concerned, large deviations from the experimental data can be seen in the low-energy (< 100 eV) region.

2.2. DDCS at fixed energies

The angular distributions at fixed emission energies, as shown in figure 2, show prominent forward–backward angular asymmetry due to the two-center effect. The enhancement of the cross section in the forward angles can be attributed to the strong attraction of the emitted electrons by receding projectiles moving in the same direction. Also, for higher-energy electrons the distributions gradually become more peaked around 75°, which is due to the binary nature of collisions. The overall shape of the distributions has been observed to match qualitatively with the CDW-EIS model calculations. The dashed lines in figures 2(a)–(c) are shown to display qualitative agreement between theory and experiment. However, the theoretical values largely overestimate the experimental values at low energies (see figures 2(a)–(c)). Quantitative agreement between theory and experiment can be found only for large energies (see figure 2(d)).

3. Single differential cross sections

The single differential cross sections (SDCS), $\frac{d\sigma}{dE}$, obtained by integrating the DDCS in an angular range of 30–150°, are shown in figure 3(a). See table 1 for the numerical values for $\frac{d\sigma}{dE}$. Similarly, the single differential cross sections, $\frac{d\sigma}{d\Omega}$, obtained by integrating the DDCS in an energy range of 10–400 eV, are shown in figure 3(b). Once again, the numerical values for $\frac{d\sigma}{d\Omega}$ have been tabulated in table 2. In both cases, the theoretical calculations reproduce the observed behaviour only qualitatively. The total cross section as obtained from the experimental data is 305.8 Mb, whereas it is 842.1 Mb as obtained from the CDW-EIS calculations.

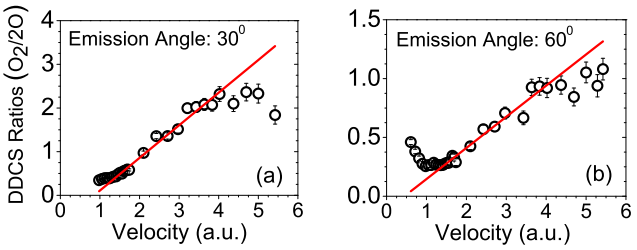

Figure 4. Ratios of molecular DDCS (for O_2) from the experiment to atomic DDCS (for O) from the CDW-EIS model, for two different angles, 30° and 60°. The solid line corresponds to the fitted straight line, $f(v) = a + bv$.

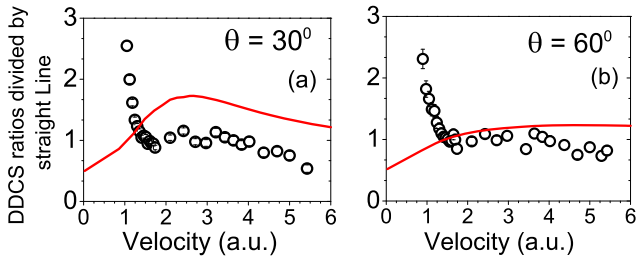

Figure 5. DDCS ratios divided by the fitted straight line at each energy value for two different angles, 30° and 60°. The solid line corresponds to the CDW-EIS calculations.

Table 2. $\frac{d\sigma}{d\Omega}$ at different angles.

Angle (deg)	$\frac{d\sigma}{d\Omega}$ (Mb sr^{-1})
30	32.58
45	23.19
60	26.21
75	41.52
90	30.10
105	13.18
120	9.22
135	10.48
150	6.21

4. Derivation of Young-type interference oscillation

For the molecular ionization process involving di-atomic molecules, a secondary electron reaching the detector cannot be tagged as an electron coming from 'this' atom or 'that' atom. Hence, the two atoms can act as two sources of coherent matter waves. These two matter waves can interfere, in the same way as two coherent light waves interfere in the case of Young-type double-slit interference, to produce a noticeable oscillatory pattern in the DDCS spectra as a function of ejected electron velocity [4, 5]. Since the effect of interference can be very small to observe accurately, it becomes necessary to divide the DDCS values obtained from the molecular target by those obtained for the atomic target under identical conditions. Accordingly, we have divided our experimental DDCS values for O_2 by two times that of O (keeping the projectile the same for both cases), to look for any such effect. However, no such effect could be observed (see figure 4).

It can be seen from figure 4 that the DDCS ratio for $O_2/2O$ increases monotonically as a function of electron velocity. This overall increase in the cross-section ratio can be parametrically represented by a straight line given as $f(v) = a + bv$. Evidently, the increase in the cross-section ratio can be removed by dividing it with this fitted straight line. This act of division was used conventionally in some earlier work [4, 5] to better reveal interference oscillation about a horizontal line. It was, however, shown that for the case of H_2, by using the measured atomic cross section [5] or a suitable effective atomic number (to take care of the mismatch of Compton profiles between molecule and atom) [10] to derive the DDCS ratio, one could get the oscillations about a horizontal line. In this work, the experimental ratio of $O_2/2O$ has been fitted with a straight line over a particular velocity range to keep the goodness of fit close to 1.0 (see figure 4).

It was then divided at each electron velocity by the corresponding value from the fitted straight line (see figure 5). We have plotted the experimental data over a velocity range of 0–5.5 au. However, no oscillatory behaviour could be seen at any emission angle (see figure 5). The solid line corresponding to the theoretical calculations displays large deviation from the experimental data.

The apparent absence of oscillations in the DDCS ratios can be explained in terms of the different molecular orbitals present in the O_2 molecule. The argument has already been presented in recent work [9, 11] in the case of impact ionization for multi-electronic as well as multi-orbital targets. Due to the triplet character of the initial molecular state, contributions from different α and β orbitals must be determined. In contrast to the case of an N_2 target, for O_2 the oscillations of DDCS ratios are much more smooth and regular (see [11, figure 7]). The ratios corresponding to the individual inner orbitals are shifted with respect to the outer shells, and when contributions from all of them are summed (as in figure 5 of this paper) no oscillations are observed. However, the presence of interference patterns may appear for each individual orbital as for the case of an N_2 target [9], for α as well as β orbitals. In fact, if theoretical DDCS ratios are obtained for each individual orbital by dividing the corresponding DDCS by the one resulting from excluding contributions coming from interference terms, oscillatory patterns are found (not shown in this paper; for a detailed explanation see [9]). This is in agreement with previous predictions, where it has been shown for N_2 that due to the different symmetries of the $1s\sigma_g$ and $1s\sigma_u^*$ and of the $2s\sigma_g$ and $2s\sigma_u^*$ orbitals, the corresponding DDCS ratios are in phase opposition [7, 9], so that oscillations cancel out when their contributions are added.

5. Summary

In summary, we studied the emission of secondary electrons from oxygen molecules in collision with bare heavy ions. The main motivation of this paper was to look for Young-type interference oscillation in the emission of electrons from multi-electronic di-atomic molecules. It has been shown, both experimentally and theoretically, in this work that there is no signature of any primary oscillation in the DDCS ratio of $O_2/2O$. This observation has been explained in terms of a multi-orbital picture from the theoretical calculations.

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