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Comparison of Experimental and Theoretical Double Differential Cross Sections of CH_4 at 250 eV Impact Energy

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In this study, experimental and theoretical double differential cross section (DDCS) data for methane-electron interaction mechanism after the impact of a 250 eV electron have been comprehensively determined for a wide energy range of the detected electron, from 50 to 225 eV. The first Born-One Coulomb wave modeling with Gamow factor has been calculated to analyze experimental DDCS results for a correct description of the electron impact ionization of methane molecule. It is found that these theoretical calculations are successful to describe the post-collision interaction effects due to the Coulomb long-range interaction between the outgoing electrons in the final state. A considerable agreement is found between experimental and theoretical results.

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1. Introduction

Electron-molecule interactions have a great interest in many areas such as, astrophysics and molecular biophysics [1–2]. Collision experiments give detailed information on the electronic structure of molecular targets and their interaction dynamics with electrons. Methane (CH_4) is an ideal target in the planetary atmosphere science, as it is one of the most abundant molecules in the atmospheres of many planets [3]. On the other side, the knowledge of electron-methane interaction dynamics is crucial for investigation of the damage of bio-molecules by electron impact [4]. In this study, the motivation is to learn, both experimentally and theoretically, about the ionization dynamics of methane molecule subjected to electron impact. This study describes DDCS measurements and theoretical First Born Approximation (FBA), corrected by Gamow factor, for methane ionization dynamics at impact with a 250 eV electron for the first time in the literature. The earlier pioneering DDCS studies for methane molecule have been reported under kinematics for 500 and 1000 eV electron impact by Opal [5] and Oda [6], respectively. DDCS measurements of electron-methane interactions have been also measured at intermediate energies [7–8]. In literature the discrepancy of DDCS data for methane molecule, used as a target, has been caused by the experimental difficulties during measurements. We report a high-accuracy set of DDCS data for methane molecule at 250 eV electron impact for almost all energies of the detected electron. In theoretical investigations, the First Born Approximation, corrected with Gamow factor, has been successfully applied to the DDCS results for the interaction of slow electrons with methane.

Section 2 discusses the experimental measurement, while first-order theoretical calculations for methane are presented in Section 3. The final section presents experimental DDCS results for methane molecule and comparison of results with the first-order theoretical calculations.

2. Materials and methods

2.1. Experiment

Detailed information of the experimental system has been published [8–11], so only a brief description will be given in this study. Summarizing, the experimental setup consists of an electron gun, methane gas jet, 180° hemispherical deflector analyzer (HDA) and a Faraday cup (FC). Figure 1 shows a schematic diagram of experimental system. The electron beam used as a projectile is produced by heating tungsten filament in the electron gun. The produced parallel electron beam (about 2 mm in diameter) is perpendicularly collided with the gas beam in the interaction region. After the collision, dependence on the energy of the outgoing electrons is analyzed by HDA for DDCS measurements. The conventional HDA is tuned to detect electrons with energy E_{det}.

After detection using the channel electron multiplier (CEM), the signal is processed by the signal processing devices to produce a signal without the external noise.

2.2. Theoretical approximation

The double differential cross section is calculated by the integration of the TDCS over the direction of one of

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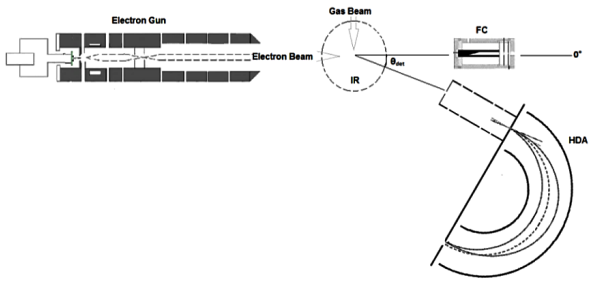

Fig. 1. Schematic diagram of experimental system. IR: Interaction Region, FC: Faraday Cup, HDA: Hemispherical Deflector Analyzer.

outgoing electrons (ejected or scattered);

$$DDCS = \frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega_{\mathrm{det}}\,\mathrm{d}E_{\mathrm{det}}}. \tag{1}$$

Here Ω_{det} and E_{det} are the solid angle and energy of detected electron, respectively. To compute the $(e, 2e)$ triple differential cross section we use the formalism developed in the frame of the one Coulomb wave model given in [12, 13]. In this formalism the TDCS can be written as follows:

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}E_{\mathrm{e}}\,\mathrm{d}\Omega_{\mathrm{e}}\,\mathrm{d}\Omega_{\mathrm{s}}} = \frac{k_{\mathrm{e}}k_{\mathrm{s}}}{k_{\mathrm{i}}}\sum_{\nu=1}^{N_{\mathrm{MO}}}\frac{A_\nu^2}{2l_\nu+1} \times \sum_{\mu=-l_\nu}^{+l_\nu}|T_\nu|^2\,\delta\left(E_{\mathrm{i}}+IP-E_{\mathrm{s}}-E_{\mathrm{e}}\right), \tag{2}$$

where k and Ω terms denote the wave vectors and solid angles of the detected electrons. E is the energy of the outgoing electron. The indexes i, s, and e denote the incident, scattered and ejected electrons, respectively. A_ν is the magnitude of contribution of each Slater orbital, used to approximate the molecular orbitals, N_{MO} is the number of the Slater orbitals. T_v is the matrix element describing the transition of the system projectile-target from the initial state to the final state [12–14].

We multiply the TDCS by the Gamow factor to take into account the post-collision interaction (PCI) effects in the final continuum state

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}E_{\mathrm{e}}\,\mathrm{d}\Omega_{\mathrm{e}}\,\mathrm{d}\Omega_{\mathrm{s}}} = \frac{k_{\mathrm{e}}k_{\mathrm{s}}}{k_{\mathrm{i}}}\frac{2\pi\xi_{\mathrm{se}}}{\exp\left(\frac{\pi\xi_{\mathrm{se}}}{2}-1\right)}\sum_{\nu=1}^{N_{\mathrm{MO}}}\frac{A_\nu^2}{2l_\nu+1} \times \sum_{\mu=-l_\nu}^{+l_\nu}|T_\nu|^2\,\delta\left(E_{\mathrm{i}}+IP-E_{\mathrm{s}}-E_{\mathrm{e}}\right), \tag{3}$$

where $\xi_{\mathrm{se}} = |k_{\mathrm{s}} - k_{\mathrm{e}}|^{-1}$. We note, that in the present work the exchange effect has been neglected, since the incident energy is important and the difference in energy between the outgoing particles is large.

3. Results and discussion

DDCSs of methane molecule were measured at impact energy (E_{i}) of 250 eV, for detected electron angles ranging from 0° to 135°. The detected electron energies (E_{det}) are within the range from 50 to 225 eV. For incident electron energy well above the methane single ionization potential ($IP = 14.25$ eV for methane), DDCS data characteristics are considerably clear. In Fig. 2, the curves (a), (b), (c) are the DDCS of the faster outgoing electron and (d), (e), (f) are the DDCS of the slower one. When the detected electron energy is high value ($E_{\mathrm{det}} = 225$, 200, 150 eV) the scattering process is dominant (Fig. 2a–c). For the detected electron with a small energy value ($E_{\mathrm{det}} = 100$, 75, 50 eV), the ionization process is dominant. DDCS data given in the Fig. 2d–f are characterized by a peak around 50° of the detected electron angle.

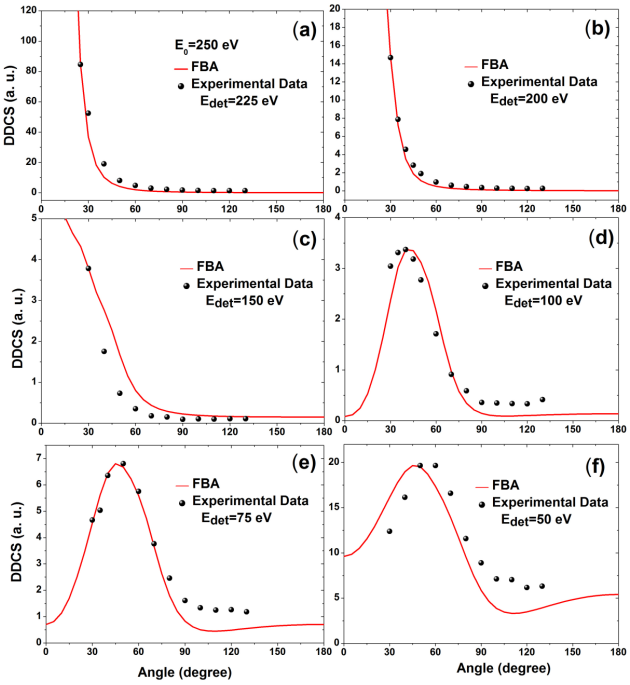

Fig. 2. Electron angular distribution from single ionization of methane by 250 eV electron impact. The experimental data are normalized to the FBA results. Solid line: Theoretical FBA calculations. Solid circles: Experimental results for detection energies of (a) 225 eV, (b) 200 eV, (c) 150 eV, (d) 100 eV (e) 75 eV, (f) 50 eV.

The range of incident energy is important to compare the experimental data with theory for correct description. In the ionization dynamics studies, high-energy region has the range of impact energies about twenty times the ionization potential (IP). The first-order theoretical calculations are required for this region. In Fig. 2, the experimental measurements are compared with the theoretical results of the First Born Approximation calculations implemented in coplanar asymmetric geometry. Theoretical results represent the sum of the DDCS for the molecular orbital $1a_1$, $1t_2$ and $2a_1$.

Theoretical calculations are generally in good agreement with the experimental results. As the energy of detected electrons increases, the First Born approximation becomes more accurate. The theory is in good agreement for the scattering energies of 225 and 200 eV, however the theory gives less accuracy for 150 eV. The same remark can be made on the results of the DDCS for the scatter-

ing energies of 50, 75 and 100 eV. It is important to note that the exchange effects and the post-collision interaction effects become important for small detected electron energies.

In the theoretical calculations, the post-collision interaction between the outgoing particles was taken into account, approximately, by means of the Gamow factor. Since the energy of the detected electrons decrease in the long range, Coulomb force between outgoing particles after collision is more effective. For this reason, the DDCS results display deviations from the theory at low detection energies. Actually, these deviations originate from the multiple interactions between incident electrons and target molecule. For more accuracy the wave function of the slow electron must contain the effect of the potential of the molecular electrons and the post collision interaction needs a more accurate description, such as using the two body Coulomb wave function, given in the BBK model.

4. Conclusions

This study presents for the first time experimental and theoretical results for electron impact ionization measurements of CH_4 DDCS. The comparison results reported in this study give a very good description of the ionization mechanisms for CH_4 by a 250 eV electron impact.

Acknowledgments

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