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Differential Cross Section of Electron Scattering from Molecular Hydrogen. II. $b^3\Sigma_u^+$ Excitation

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Differential cross section(DCS) for the electron-impact $H_2(b^3\Sigma_u^+)$ excitation has been measured in the incident energy range from 12 to 60 eV and in the angular range from 10° to 130°. The electron transmission efficiency of the energy analyzer was calibrated using the secondary electron emission cross sections from N_2 molecule. The inelastic DCS is normalized to the absolute H_2 elastic DCS. Integral cross section is derived from the measured DCS. Measured DCS is compared with other experimental and theoretical results.

§1. Introduction

Electron-molecular hydrogen collision is the basic problem in the theory of molecular collision. Therefore, many theoreticians have studied the elastic and inelastic collision processes in this system. Reliable collision cross section data on e-H_2 are also needed in the study of the planetary and the earth's upper atmosphere, of gaseous discharge and of modeling of plasmas in thermo-nuclear reactors. On the other hand, experimental studies of these processes have been made only fragmentarily[1] so far. In our laboratory, systematic measurements of the DCS on e-H_2 collisions have been planned. We have already reported the elastic DCS[2] for H_2. For the stringent test of the collision theories, the b state [$H_2(b^3\Sigma_u^+)$] excitation is a suitable process because it is excited only through the electron exchange collision. In this report, absolute DCS for the b state excitation is given for low energy incident electrons and is compared with other experimental and theoretical results.

A hydrogen molecule excited into the b state dissociates into two H(1s) atoms with considerable kinetic energies. The cross section for this process can be obtained by the direct measurement of the dissociation products. Alternatively, measurement of the scattered electrons, which have excited H_2 into the b state, should give the same cross section. Due to the difficulty in the former method of the direct detection of H(1s) atoms from this process, the latter method is more reliable for the cross section measurement of the b state excitation. The electron energy loss spectrum from this process is a broad and flat feature. Since more than half portion of the energy loss spectrum for this process has no overlap with those of other electronic features, accurate measurement of the DCS can be expected.

Corrigan[3] determined the integral excitation cross section by measuring the adsorption rate of dissociation fragments on molybdenum trioxide. The method used by Corrigan belongs to the former type experiment. The cross section reported by Corrigan includes contribution of the cascade effects from the upper $^3\Sigma$ states as was discussed in this paper. Recently, Hall and Andric[4] measured the DCS(10.5 eV, 20°–120°) by a crossed beam method in which a mixture of He and H_2 was used as target. Absolute values were determined by comparing the scattered electron intensities from the He 2^3S state excitation with those from the H_2 b state excitation.

As will be explained later, the transmission efficiency of our analyzer was determined by measuring the relative intensities of secondary electrons from N_2 molecules. The absolute DCS for the b state excitation were determined in the incident electron energy range from 12 to 60 eV and in the scattering angular range from 10° to 130°. Measured values are compared with those of other experimental

results.

A large number of theoretical works in various types of calculation method have been reported so far. The cross section has been studied by Trajmar *et al.*[5] and Cartwright and Kuppermann[6] in the Ochkur-Rudge approximation(OR), by Chung *et al.*[7] in the Born-Rudge approximation(BR), by Resigno *et al.*[8] in the distorted wave random phase approximation(DW-RPA) and by Filflet and McKoy[9] in the distorted wave approximation(DW). Calculations in the close coupling method(CC) by Weatherford,[10] by Schneider and Collins,[11] in the hybrid close coupling R-matrix method(CC-RM) by Holley *et al.*,[12] in the Schwinger multichannel variation method(SMV) by Lima *et al.*[13] and in the R-matrix method(RM) by Baluja *et al.*[14] were also carried out for this process. Typical calculated results are compared with the measured cross sections in §3.

§2. Experimental

The experimental apparatus used was described in an earlier report.[2] In brief, the energy selected electrons from a hemispherical monochromator are focussed onto a molecular beam at right angles. Inelastically scattered electrons from molecules are energy analyzed by the same type of analyzer and detected by an electron multiplier. The apparatus was operated with overall energy resolution of about 100 meV and incident electron current of 1–10 nA. Density of the molecular beam effused from a multichannel capillary array was controlled by adjusting the pressure behind the capillary array using a fine needle valve and monitored by measuring the background pressure of the collision chamber. Pre-purified H_2(99.95%) was used in this experiment. The analyzer can be rotated around the collision center from $-20°$ to 130°. The magnetic field around the apparatus was reduced to about 10 mG by a mu-metal can and a three dimensional Helmholtz coil.

Measurements have been carried out in the following way. First, the electron transmission efficiency of the electron analyzer is calibrated in the range between the b state feature and the elastic peak in the energy loss spectrum. This method was developed by Pichou *et al.*[15] who determined the transmission efficiency using an energy distribution of the continuum electrons in the ionization of helium by electron impact. For an accurate detector calibration, it is convenient to use the differential secondary electron emission cross sections (DSEECS) which have the following characters. Firstly, those emitted electrons have almost a flat feature in the energy spectrum. Secondly, magnitude of those cross sections are large enough for this purpose. Taking these points into account, the DSEECS for N_2 molecules which were reported by Opal *et al.*[16] and Shyn[17] were used in this study. An energy spectrum of the scattered electrons from molecules can be divided into two main parts. A part of the energy range from 0 eV to $(E_1 - IP)/2$ mainly consists of ejected electrons and the rest mainly consists of inelastically and elastically scattered electrons where E and IP are the impact energy and the ionization potential of the target molecule, respectively.

Procedure for the calibration of the detector system in a desired energy range, say, from E_0 to E_1, is as follows. E_1 is the residual energy of the incident electrons with E_0 after the excitation of the molecule. Electrons of energy $E(0)$ are crossed with the N_2 molecular beam, where $E(0)$ is one of the electron impact energies where the secondary electron energy spectrum has been determined in refs. 16 and 17. Continuum electrons from N_2 molecules in the energy range from E_0 to E_1 are energy analyzed and detected by the electron energy analyzer at a fixed angle (typically 60°). Adjusting the potentials applied on the electron optics in the analyzer system, measured secondary electron emission spectrum from N_2 molecules are compared with the standard DSEECS.[16,17] The relative electron transmission efficiency of the analyzer system is thus determined.

Holding the potentials applied on the electron optics in the analyzer system, electron impact energy is shifted from $E(0)$ to E_0 which is a desired impact energy. The absolute DCS values of the inelastic electron scattering from H_2 molecules can be determined from the ratio of the inelastically scattered electron intensity to the elastically scattered one multiplied by

the absolute values of the elastic H_2 DCS.

Resigno *et al.*[8] reported the agreement between the envelope of their calculated Franck-Condon factor(FCF) distribution and the shape of the measured energy loss spectrum for the b state excitation. In the present measurement, the electron intensities scattered from the b state excitation are integrated over the electron energy loss range from 7.0 eV to 10.38 eV at each impact energy ($E \geq 15$ eV) and each scattering angle so as to count the scattered electron intensities of the lower half area of this feature in the energy loss psectrum. The lower limit (7.0 eV) of the integral was taken from ref. 13. Taking into account the profile of the FCF distribution for the b state excitation, we choose the upper limit (10.38 eV) of the integral so as to divide the energy loss feature into two equal parts in intensity. For lower incident electron energies ($E \leq 13$ eV), ratio of the scattered electrons into the upper part (10.38 eV$-E_0$) to those into the lower part (7.0 eV-10.38 eV) of the energy loss range is determined by integrating the FCF profile. The number of whole scattered electrons is derived using this ratio and the number of electrons scattered with energy loss between 7.0 eV and 10.38 eV. This procedure for low incident energies is not expected to give results with high accuracy, but it is the best we can do. Background correction is also made for the spurious counts of the detector. Measurements are carried out in the incident electron energy range from 12 to 60 eV and in the angular range from 10° to 130°. A typical energy loss spectrum is shown in Fig. 1.

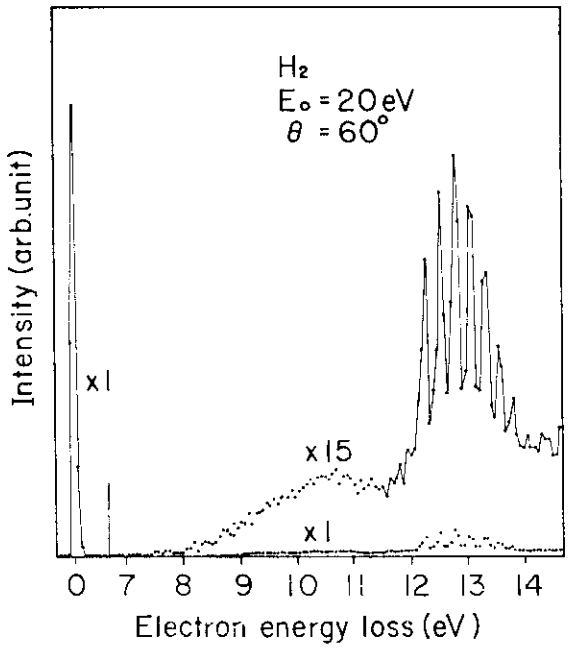

Fig. 1. Energy loss spectrum of H_2 including the elastic peak, the $b^3\Sigma_u^+$ continuum and a part of the $B^1\Sigma_u^+$ and $C^1\Pi_u$ levels, at 20 eV of incident electron energy and at 60° of scattering angle.

§3. Results and Discussion

The uncertainties of the measured DCS values come from the estimation of the target density(10%), incident electron current(3%) and the electron transmission through the electron energy analyzer system(27%). The resultant experimental error of the DCS values is estimated as 37% or less which include those due to the integration of the number of scattered electrons over the relevant energy range(10%) and of the H_2 elastic DCS(20%). The values of DCS measured are summerized in Table 1. The integral cross section σ_i which is derived by integration of the measured DCS after the extrapolation to forward and backward scattering angles is also shown in the table. In Fig. 2 the determined DCS values are compared with the theoretical results and the experimental results of Hall and Andric. At 12 eV of electron energy, our DCS values show monotonous increase with increasing scattering angle and are in reasonably good agreement with results of Hall and Andric. In the energy region measured in this work, we can not find reliable experimental DCS data any more to be compared with the present results.

As can be seen from Fig. 2, recent theoretical results of Lima *et al.* (SMV) are in excellent agreement with the present results at 15, 20 and 30 eV. However, in the energy region near the excitation threshold, the results of Lima *et al.*(SMV) and of Fliflet and McKoy(DW) give some pronounced deviation from the experimental results at the extremes of their angular range. The calculations of Trajmar *et al.*(OR) and of Fliflet and McKoy(DW) agree reasonably well with the present results in the higher energy range (40, 60 eV). The calculated results of Weather-

Table 1. Differential and integral cross sections for the excitation of the $b^3\Sigma_u^+$ state in H_2 by electron impact.
DCS(10^{-18} cm^2/sr)

E_0(eV) θ(deg)	12	13	15	17	20	30	40	60
10				6.08	5.60	3.26	1.50	1.08
15			4.59		4.23	2.93	1.32	1.02
20	1.52	1.68	4.24	4.62	4.54	2.68	1.21	0.876
30	1.62	1.51	3.65	4.57	3.44	2.37	1.47	0.980
40	2.17	1.68	2.68	3.61	3.09	2.26	1.46	0.898
50	2.05	1.68	2.89	3.42	2.86	1.81	1.33	0.626
60	2.29	2.74	2.85	3.37	2.86	2.02	1.19	0.464
70	2.34	2.49	3.02	3.09	2.46	1.67	0.858	0.356
80	2.45	2.93	3.50	3.55	2.23	1.72	0.614	0.192
90	3.12	3.12	3.79	3.44	2.92	1.68	0.436	0.158
100	3.47	3.64	4.04	3.60	3.28	1.44	0.360	0.099
110	3.40	4.70	4.60	3.53	4.14	1.40	0.256	0.0826
120	5.00	5.45	5.75	4.45	4.56	1.46	0.229	0.0678
125	5.46							
130		6.91	6.94	5.06	4.95	1.27	0.218	
σ_i	40.0	51.8	60.4	53.7	48.4	21.2	8.21	3.80

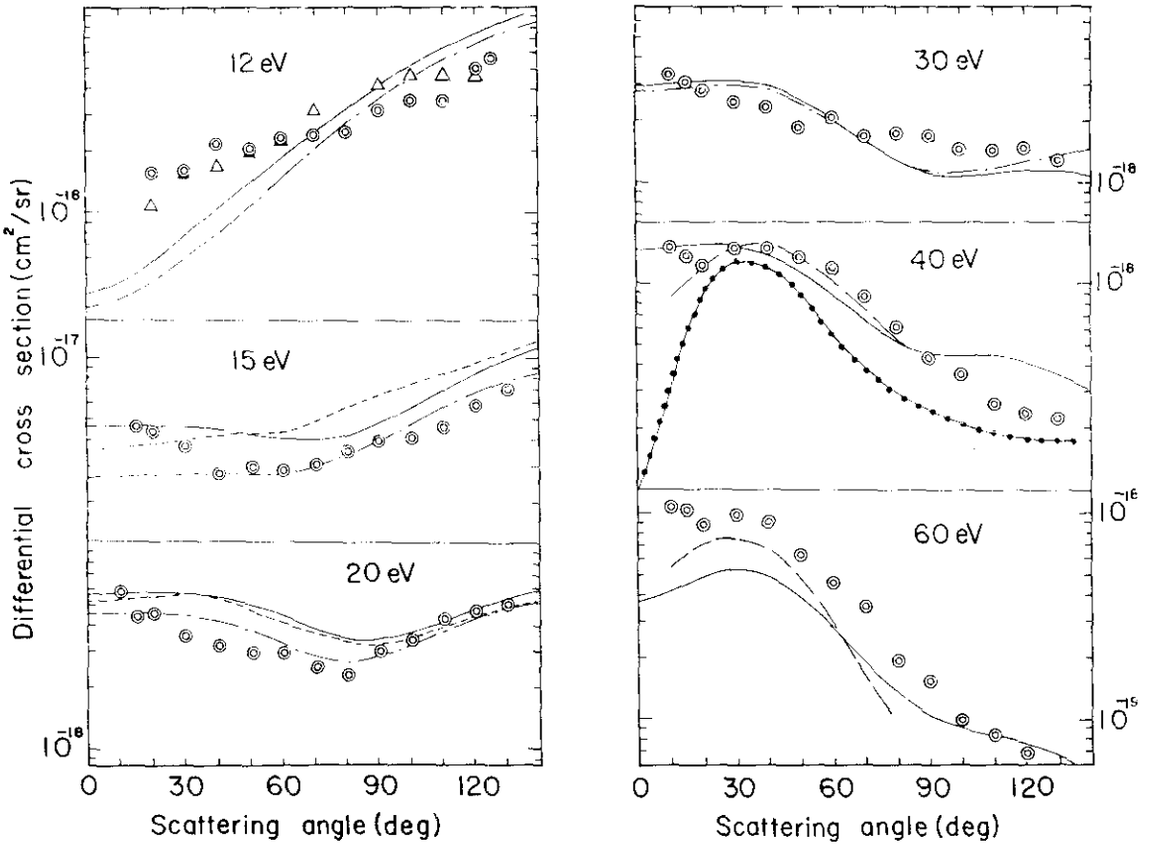

Fig. 2. Differential cross sections for the H_2 $b^3\Sigma_u^+$ excitation in the energy range between 12 and 60 eV of electrons. Experimental: ◎: present results, △: Hall and Andric. Theoretical: ----: Resigno *et al.* (DW-RPA), —: Fliflet and McKoy (DW), ——: Lima *et al.* (SMV), ———: Trajmar *et al.* (OR), •••• : Weatherford(CC-SCEA).

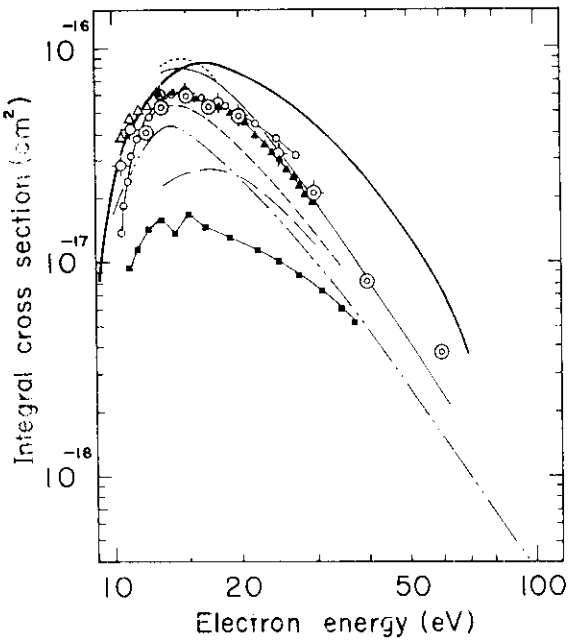

Fig. 3. Integral cross sections for the H_2 $b^3\Sigma_u^+$ excitation. Experimental: ⊙: present results, △: Hall and Andric. ——: Corrigan. Theoretical: ⊹: Lima *et al.*(SMV), ▲▲▲ : Schneider, and Corrins(CC), ●●● : Weatherford(CC-SCEA), ——: Holley *et al.*(CC-RM), ⊸⊸⊸: Baluja *et al.*(RM), —: Fliflet and McKoy(DW), ·····: Resigno *et al.*(DW-RPA), ----: Chung *et al.*(BR), -------: Cartwright and Kuppermann(OR).

ford(CC-SCEA) show angular behaviour different from the experimental results at forward scattering angle at 40 eV.

The integral cross section derived from the measured DCS is shown in Fig. 3 with the other experimental and some theoretical values. The present results show a broad maximum around 15 eV and decrease monotonously with increasing electron energy. Agreement between the present results and those of Hall and Andric is good within experimental errors. Measured results of Corrigan give higher values than the present results by about factor 2 at higher energies and approach to the present results at energies lower than 13 eV. The difference between those two experiments at higher energies can be attributed to the cascade effect from the upper states and the contribution of neutral products from the other excitation levels. Recent calculations of Lima *et al.* in SMV, Schneider and Collins in CC and of Baluja *et al.* in RM have given excellent predictions to the present results. The calculations of Cartwright and Kuppermann in OR and of Fliflet and McKoy in DW also reproduce the present results reasonably well at higher electron energies. The calculations of Holley *et al.* in CC-RM give considerably lower values than the present results and the more recent theoretical results.

§4. Summary

The differential and the integral cross sections for the b state excitation are measured using a crossed beam and the relative flow method. There is a good agreement between the present results and those of earlier experiment by Corrigan at lower electron energies. The cross sections measured by Hall and Andric are in good agreement with this work. Among many theoretical cross sections for the b state excitation, the recent results of Lima *et al.* in SMV, of Schneider and Collins in CC and those of Baluja *et al.* in RM calculation are in excellent agreement with the present results at electron energies higher than 15 eV. The theoretical results of Fliflet and McKoy in DW and those of Cartwright and Kuppermann and Trajmar *et al.* in OR give reasonably good predictions for the present results in higher energy region.

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