Single and double ionization of H_2 by He^{2+}

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Cross sections for the nondissociative single ionization and double ionization of H_2 by He^{2+} projectiles in the range of 125–750 keV/amu are reported. The results are compared to impact-parameter calculations and to measurements with He^+ projectiles. The direct double-collision process is found to be the important contributor to double ionization in this range of energies. The single-ionization cross section, when compared to proton bombardment, does not scale as Z^2.

I. INTRODUCTION

Recent studies[1–4] of the double ionization of helium by He^{2+} projectiles have shown that double ionization occurs mainly by two projectile-electron interactions (double collisions) when the projectile velocity is less than 1000 keV/amu. At much higher velocities it is expected that double ionization occurs mainly by the shakeoff process. At intermediate velocities both proccesses contribute.[5]

In the double-collision regime, the two target electrons have been treated theoretically[6,7] with the independent electron approximation (IEA). If the probability of removing a single electron by a projectile-electron interaction is known, the single- and double-ionization cross sections can be calculated via the IEA and used to investigate general properties of the collision. The probability of removing a single electron has been found and tabulated for the semiclassical Coulomb approximation (SCA).[7,8]

This article reports on the double ionization σ^{2+} and nondissociative single ionization σ^+ of H_2 by He^{2+} projectiles and compares the results to similar measurements with a helium target and to He^+ bombardment. The IEA is used to investigate the dependence of the collision on the projectile charge and to investigate the double-ionization mechanism in the collision range of 125–750 keV/amu.

II. EXPERIMENTAL PROCEDURE

A pulsed beam of He^+ ions is extracted from the University of Georgia Van de Graaff accelerator (0.5–3.0 MV), momentum analyzed, and passed through a gas stripping cell. The beam is then focused by a magnetic quadrupole lens into an electrostatic deflection cell that separates the He^{2+} component from the primary beam and directs the He^{2+} into the collision chamber.

The apparatus used to measure the double- and single-ionization cross sections is the same as used previously.[9] To detect the H_2 double-ionization events, two hemispherical analyzers placed on opposite sides of the He^{2+} beam at ±90° record the fragments in coincidence. Each H^+ fragment has about 10 eV of energy arising from the mutual Coulomb repulsion within the dissociating ion. The time of flight from the collision region to the detector and the energy are both measured in order to separate the H^+ ions from background ions that are formed at the same energy.

In order to detect the nondissociative single-ionization events, one of the hemispherical analyzers is removed and a set of parallel plates is installed in the collision region. $H_2{}^+$ ions formed by collisions are accelerated toward the remaining analyzer by a small voltage placed on the back plate. The front plate has a small aperture in it to allow the ions to pass to the analyzer.

The apparatus used in the single-ionization measurements was calibrated by measuring the single ionization of helium by protons and normalizing the results to the recommended values of Rudd *et al.*[10] The uncertainties are a combination of the statistical error in the present work and the uncertainties associated with the values of Rudd *et al.* The method used to calibrate the double-ionization cross sections is described in Ref. 11.

In earlier measurements of the double ionization of H_2, uncertainties in the absolute (but not relative) cross sections were large because target gas pressure, detector efficiency, and the transmission functions of the two analyzers used in the coincidence mode could not be measured directly. One major uncertainty arose from the kinematic spread in the relative directions and energies of the two ions ejected in the double-ionization process be-

TABLE I. Cross sections for single and double ionization of H_2 by He^{2+} projectiles.

keV/amu	σ^+ (10^{-16} cm^2)	σ^{2+} (10^{-18} cm^2)
125	5.34±0.32	12.4±2.0
187.5	4.43±0.27	9.95±1.7
250	3.74±0.22	6.99±1.12
375	2.98±0.18	3.94±0.63
500	2.39±0.14	2.49±0.40
625	2.05±0.12	1.70±0.27
750	1.75±0.11	1.27±0.20

TABLE II. Cross sections for single and double ionization of H_2 by He^+ projectiles.

keV/amu	σ^+ (10^{-16} cm^2)	σ^{2+} (10^{-18} cm^2)
125	2.48±0.13	11.1±1.8
187.5	1.92±0.12	5.42±0.87
250	1.59±0.10	3.59±0.58
375	1.36±0.08	1.97±0.32
500	1.12±0.08	1.17±0.19
625	0.831±0.053	0.851±0.136
750	0.762±0.046	0.678±0.108

cause of the thermal motion of the target molecules. Another arose from target-gas-density estimates based on gas flow and pumping speed.

We have recently made Rutherford scattering measurements of protons on argon to establish the target gas density with greater accuracy. The fitting procedures described in Ref. 11 do not involve coincidence measurements and the difficult problem of calculating the combined effect of two analyzers operating in the coincidence mode is eliminated. The new calibration procedures determine that our previous absolute values of the double-ionization cross sections are too small by a factor of about 12. The relative values of the cross sections as reflected in the energy dependence are unaffected. The errors listed in Tables I and II for double ionization reflect the 15% uncertainty described in Ref. 11 plus the reproducibility of six or more measurements made at each beam energy.

III. RESULTS AND DISCUSSION

The single- and double-ionization cross sections of H_2 by He^{2+} projectiles are shown in Figs. 1 and 2 and are tabulated in Table I. The data for He^+ on H_2 are contained in Table II and are also shown in the figures. The σ^+ data of Table II are reproduced from Ref. 12, while the σ^{2+} data are the results of the improved calibration procedures described above and differ from values published earlier.[12]

The solid curves in Figs. 1 and 2 represent the results of calculations based on the independent electron approximation. In essence, the probability $P(b)$ of a projectile with impact parameter b removing a single electron by ionization of the molecule is calculated as a first step. In order to find the cross sections, the probability is integrated over all impact parameters according to the following relationships:

$$\sigma^+ = 2\pi \int_0^\infty 2b\, P(b)[1-P(b)]db$$

and

$$\sigma^{2+} = 2\pi \int_0^\infty b\,[P(b)]^2 db \ .$$

The values of $P(b)$ used to calculate the cross sections must be scaled according to the effective charge of the projectile. In this work, the projectile charge scaling for He^+ projectiles was completed by calculating the ratio of

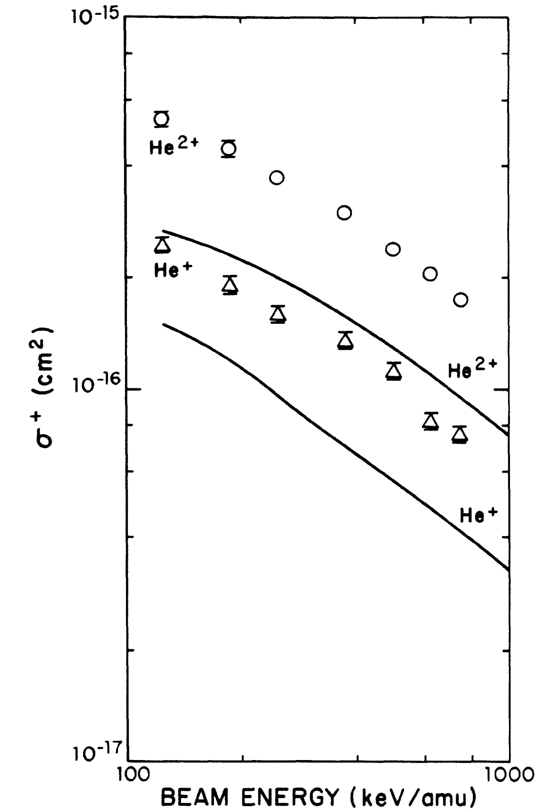

FIG. 1. Single-ionization cross sections of H_2 by He^{2+} and He^+ projectiles. Solid lines are impact-parameter calculations.

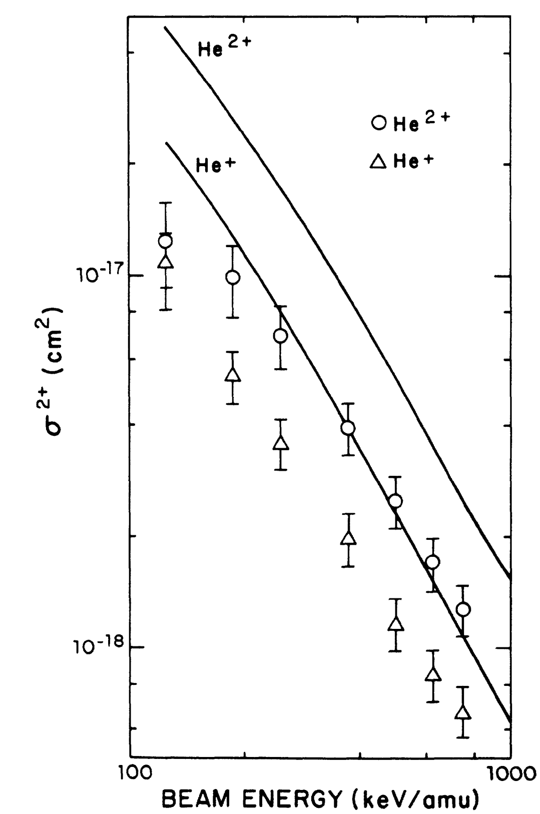

FIG. 2. Double-ionization cross sections of H_2 by He^{2+} and He^+ projectiles. Solid lines are impact-parameter calculations.

single-ionization cross sections for He^{2+} and He^{+} bombardment and assuming a Z^2 dependence. This yielded an effective Z of 1.3 for He^{+} for single ionization. For double ionization, where the energy transfer in a collision is greater than for single ionization, the effective Z of He^{+} is expected to be larger.[13,14] Ratios of double-ionization cross sections were calculated and a Z^4 dependence was assumed. An effective Z of 1.6 resulted. The effective charge of the H_2 target was found by the same method as used for a helium target.[8] The average ionization potential (25.5 eV) of the ground-state σ_g orbital is set equal to $13.6Z^2/1^2$ and yields $Z=1.37$.

Measurements and calculations similar to those reported here for a H_2 target were also carried out in our laboratory with a helium target. Since the ionization of helium has been well studied, it serves as a check on our scaling procedures and experimental results. The data obtained with the helium and hydrogen targets are comparable. In each case the measured single-ionization cross section is underestimated by the model calculation by a factor between 1.5 and 2.0. The measured double-ionization cross sections for the H_2 target fall below the model predictions as they do for the He target. It is possible to improve the fit by adjusting the effective charge of the target molecule, but that was not done in this work.

It is interesting to observe that the velocity dependencies of the model calculations and the data are comparable. Comparisons can be made also between the nondissociative single ionization of H_2 by protons and He^{2+} at 750 keV/amu. This comparison yields a ratio of cross sections for He^{2+}/H^{+} of 3.60 ± 0.18, showing that there is not a simple Z^2 dependence at this energy. Olson[15,16] calculated this ratio for a helium target using his classical trajectory Monte Carlo method and obtained 3.76 ± 0.12. Our helium measurements yielded 3.69 ± 0.18. In the same vein, we recently reported on the non-Z^2 dependence of the single ionization of H_2 by electrons and protons.[9] In the present data the ratio of double-ionization cross sections for He^{2+} and H^{+} projectiles at 750 keV/amu is 9.6 ± 2.2. This result is closer to a Z^3 dependence than to a Z^4 dependence on projectile charge.

If one assumes that double ionization occurs by a direct double-collision process, it can be shown,[1,6] that σ^{2+} is directly proportional to $(\sigma^{+})^2$. Dubois and Manson[1,6] analyzed single- and double-ionization cross-section measurements for a helium target in terms of the independent electron model. It is assumed that the ionization probability is given by the simple form $P(b)=P(0)e^{-b/R}$, where R is a characteristic interaction distance. For proton impact in the range 50–500 keV a constant R was found which was approximately 60–70% larger than the mean radius of the 1s orbital of helium. The data for He^{2+} impact[1] supported the same conclusions and led to the same value of R. Our helium target measurements at high energies where charge capture is negligible yield values of R in agreement with those of Dubois.

In the present work with an H_2 target the ratio of σ^{2+} to $(\sigma^{+})^2$ is fairly constant over the range of energies studied. Following the method of Dubois, a characteristic interaction distance can be deduced. Figure 3 shows the results of such an analysis. The He^{2+} data at 125, 187.5, and 250 keV/amu were corrected for double ionization by transfer ionization.[17] The calculations of R for the He^{+} beam were corrected by a factor of $(1.6)^2/(1.3)^2$ to account for the different effective Z value of He^{+} in single and double ionization, but corrections were not made for transfer ionization.

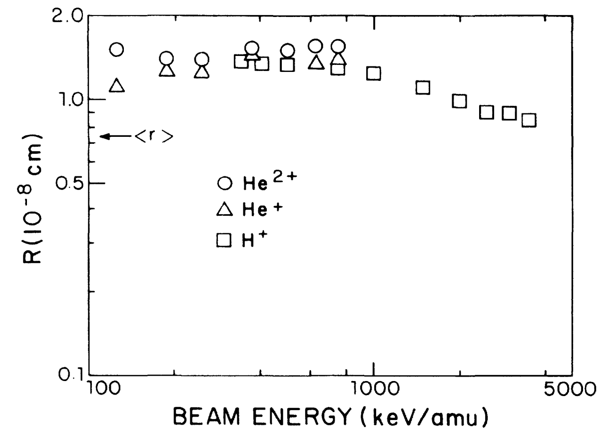

FIG. 3. Characteristic interaction distances for the double ionization of H_2 by He^{2+}, He^{+}, and H^{+} projectiles. The mean radius of H_2 is indicated by $\langle r \rangle$.

Also included in Fig. 3 are R values deduced from data reported[11] from our laboratory for protons incident on H_2. Overall, the H_2 data show the same trends as the results of Dubois[1] for a helium target, but the values for H_2 are larger by a factor of about 1.8.

In order to complete the comparisons the mean size of the $1\sigma_g$ orbital of the H_2 molecule was calculated. This was done by integrating the H_2 electron densities given recently by Moszyński and Szalewicz.[18] The value calculated is shown in Fig. 3. As in the case of the helium target data, the measured values for the interaction distance are larger than the mean size. In this case the interaction distance is about twice the mean size of the $1\sigma_g$ orbital.

In summary, our measurements support the thesis that for double ionization of H_2 by He^{2+} projectiles at energies below 1000 keV/amu, the most important process is a two-step direct, double-collision process. Only at the highest energies should other processes such as shakeoff be considered.

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