PHYSICAL REVIEW A **VOLUME 32, NUMBER 3** **SEPTEMBER 1985**

Double ionization of H_2 caused by two sequential projectile-electron collisions

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(Received 6 May 1985)

The impact-parameter calculations of Hansteen *et al.* [J. Phys. B **17**, 3545 (1984)] for *K*-shell ionization are used to predict the cross sections for the double ionization of H_2 and He by H^+ and D^+ projectiles as a function of projectile velocity. The calculated values in the case of the H_2 target are typically a factor of 12 lower than the measured values, but the calculations and measurements show similar velocity dependencies. The results indicate that for projectile energies less than 1 MeV/amu, the double-ionization process of H_2 occurs mainly by two independent interactions between the electrons and projectile. For the He target, the calculated and measured values for the double-ionization cross section are much closer in magnitude, but the calculations predict a more rapid falloff with projectile velocity than is observed.

A recent publication[1] from our laboratory reported on the cross sections for double ionization of H_2 by fast H^+ and D^+ projectiles. Projectile energies ranged from 0.08 to 3.5 MeV/amu, and the H_2 internuclear axis was fixed in a horizontal plane ($\phi = 0°$) at either 90° or 30° relative to the beam direction. It was shown that the Bethe-Born approximation did not give a qualitative fit to the data for projectile velocities less than about 10 atomic units. It was assumed that this indicated that a two-step or double-collision process was the important interaction for double ionization at the lower velocities, and a second Born term would be needed. In this model, the projectile interacts independently with the two electrons of H_2 to produce the double ionization. Knudsen *et al.*,[2] in their work on the double ionization of helium, used a parameter first introduced by Bohr[3] to specify our collision regime as an intermediate region; in our work the parameter κ falls in the range $0.1 \lesssim \kappa \lesssim 1$, where $\kappa = 2qv_0/V$, q is the projectile charge, v_0 the electron velocity in the first Bohr orbit, and V the projectile velocity. In this intermediate region the ion-electron interaction becomes stronger relative to the electron-electron correlation, and the double-collision process is expected to be the important interaction.

A relatively simple impact-parameter model can be used to test our data in order to estimate the importance of the double-collision mechanism. In the impact-parameter model, the cross section for double ionization is given by

$$\sigma = 2\pi \int_0^\infty P_{v1}(b) P_{v2}(b)\, b\, db \ ,$$

where b is the impact parameter, $P_{v1}(b)$ is the probability of removing the first electron, and $P_{v2}(b)$ is the probability of removing the second electron. We have assumed straight-line trajectories for the projectiles and used the tables of Hansteen, Johnsen, and Kocbach,[4] as suggested by McGuire and Weaver,[5] in order to find the Coulomb ionization probabilities. Following the work of Hansteen and Mosebekk,[6] Kaminsky and Popova,[7] and Sidorovich and Nikolaev,[8] it was assumed that $P_{v1}(b) = P_{v2}(b)$, and that the Slater rules[9] could be used to find the effective Z of the target from the mean binding energy of its two electrons (25.6 eV). This procedure yields an effective Z of 1.37. The integration was done numerically using Simpson's rule.

The calculated cross section is a total cross section, whereas the measured values are differential in the angle of orientation of the molecular internuclear axis. The measurements[1] indicated that the cross section is isotropic with regard to molecular orientation. Therefore, the calculated values were multiplied by the solid angle acceptance factor of the detectors in order to compare calculations and data. In order to account for the target being a molecule rather than an atom, it was also assumed that the H_2 target has twice the radius of an atom with a mean binding energy of 25.6 eV. This introduces a factor of 4 in the calculation of the cross section. With all of the assumptions the calculated values are smaller than the measured values by a factor of about 12 for projectile energies in a range of energies near 0.5 MeV/amu.

The smooth line in Fig. 1 is drawn through the calculated

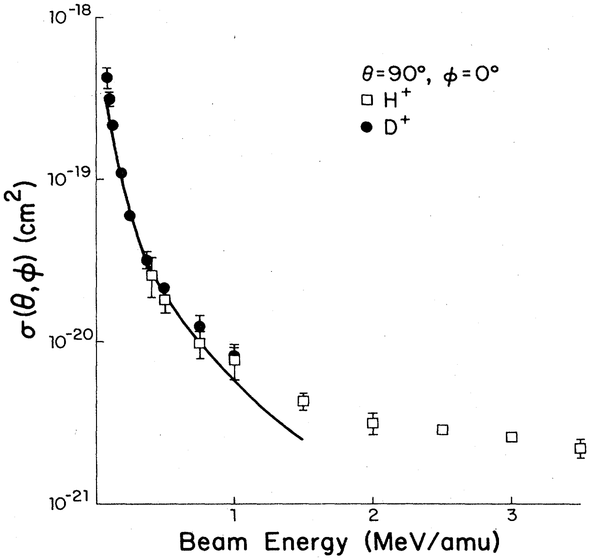

FIG. 1. The estimated cross sections for the double ionization of H_2 by H^+ and D^+ projectiles. The internuclear axis of the H_2 molecule lies in the horizontal plane ($\phi = 0°$) and is oriented at 90° relative to the beam axis. The smooth line is an impact-parameter calculation normalized at 0.5 MeV/amu.

values that have been multiplied by a factor of 12. The two measured points at 0.08 and 0.10 MeV/amu are slightly higher than the corrected calculated values, presumably because of charge capture by the projectile. For high projectile velocities, the increase in the measured cross section is assumed to indicate the relative importance of the shakeoff process. The tables of Hansteen *et al.*[4] do not extend beyond 1.5 MeV/amu for the parameters that we have used. The trend of the data below 1 MeV/amu does match that predicted by a double-collision model.

Shah and Gilbody[10] measured the single- and double-ionization cross sections for helium bombarded by H^+ projectiles in the same projectile energy range as considered here. The H_2 double-ionization cross sections discussed here fall off faster with increasing projectile velocity than do the He double-ionization cross sections. The tables of Hansteen *et al.*[4] can be used to predict both the single- and double-ionization cross sections of helium in the range of 0.2–2.0 MeV/amu projectiles. The single-ionization predictions are a factor of 2 smaller than the measured values, but the decline of the cross section with increasing projectile velocity is correctly predicted. The double-ionization predictions are closer in magnitude to the measured values than in the case of single ionization; however, the predicted values fall off faster with increasing projectile velocity than do the measured values.

In summary, the double-collision model and its prediction of the double-ionization cross section as a function of projectile velocity in the range of 0.1–1 MeV/amu gives qualitative agreement with the measured values of the double ionization of H_2, but does not account as well for the He data. This suggests that in this projectile energy range, double collisions play a more important role in the double ionization of hydrogen than of helium. It must be cautioned, however, that the scaling as described by Kocbach[11] for the Hansteen *et al.*[4] tables has been pushed to the extreme and makes conclusions tentative.

We thank Joseph Macek for suggesting that we compare our data to the impact-parameter calculations.

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