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Low-energy electron capture by B^{4+} ions from hydrogen atoms

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Using a merged-beam technique, the absolute, total electron-capture cross section has been measured for collisions of B^{4+} ions with hydrogen (deuterium) atoms at collision energies between 60 and 1200 eV/amu. The data are compared to two semiclassical coupled-channel molecular-orbital calculations, which differ by 30% with respect to each other over the entire energy range, and to two previous measurements at higher energies that differ by up to a factor of 2. [S1050-2947(98)04703-9]

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I. INTRODUCTION

Current studies of electron-capture processes are motivated by the fact that they constitute reaction channels of fundamental importance in plasma environments, such as in fusion devices and stellar plasmas. With respect to fusion energy research, electron-capture cross sections at eV/amu energies are needed for the modeling and diagnostics of the edge or scrape-off plasma. The status and critical assessment of the atomic data base relevant to magnetic fusion for collisions of Be^{q+} and B^{q+} ions with H, H_2, and He can be found in the literature [1].

Low-energy theoretical data for $B^{4+}+H$ collisions were first supplied by Shimakura, Suzuki, and Kimura [2], who calculated the total and partial cross sections using a fully quantal molecular method below 30 eV/amu and a semiclassical method above 15 eV/amu. The calculations use close-coupled molecular orbitals including rotational couplings and electron translation factors. Capture is predicted to occur in three (strongly coupled) channels, namely, $B^{3+}(1s3s)$, $B^{3+}(1s3p)$, and $B^{3+}(1s3d)$ [2]. More recently, Fraija, Allouche, and Bacchus-Montabonel [3] used a semiclassical treatment with *ab initio* molecular potentials to calculate the total and partial cross sections and found a total cross section significantly larger than the prediction of Shimakura, Suzuki, and Kimura [2]. Previously, it has been observed that low-energy close-coupled calculations are extremely sensitive to the molecular potentials and the subsequently derived couplings [4], and could lead to the discrepancy just mentioned. Both calculations claim reasonable agreement with existing experimental data. However, previous hydrogen furnace measurements by Crandall, Phaneuf, and Meyer [5] and Gardner *et al.* [6] differ by up to a factor of two and only extend down to 2000 eV/amu. More experimental work is reported in the literature, but these results are only for collision energies exceeding 16 keV/amu [7]. To provide a better test for theory, additional measurements at lower collision energies are presented.

II. EXPERIMENT

Measurement of the electron-capture cross section of the $B^{4+}+H$ system was performed using the Oak Ridge National Laboratory (ORNL) ion-atom merged-beam apparatus, which has been comprehensively described previously [8,9]. This apparatus is depicted schematically in Fig. 1. By merging two fast beams of neutral atoms and multiply charged ions, a large dynamic range of collision energies becomes available [9], allowing access from keV/amu down to meV/amu collision energies. In the present investigation, a variable-energy (60–105 keV) B^{4+} beam was merged with an 8-keV and 10-keV D beam, and the total electron-capture cross section was measured in the energy range of 60–1200 eV/amu. Deuterium was used instead of hydrogen to maximize the angular acceptance of the apparatus [8,10]. Isotope effects due to differences in trajectories [11] are not expected at these energies. Such isotope effects are known to exist for ions of similar charge, e.g., $Si^{4+}+H(D)$ [12], but for collision energies below 1.0 eV/amu. For ions with higher charges, isotope effects are predicted to occur at higher collision energies [13].

The B^{4+} beam is produced by the ORNL CAPRICE electron cyclotron resonance (ECR) ion source with an intensity of approximately 1 μA, a diameter of 2–4 mm [full width at half maximum (FWHM)] and a divergence less than 0.25°. Due to the Stark mixing by strong extraction fields present in the source, the hydrogenlike ion beam is expected to be in the ground state [14]. A fast neutral ground state D atom beam is obtained by photodetachment of an 8- or 10-keV D^- beam using a 1.06-μm cw Nd:YAG laser. The D^- beam

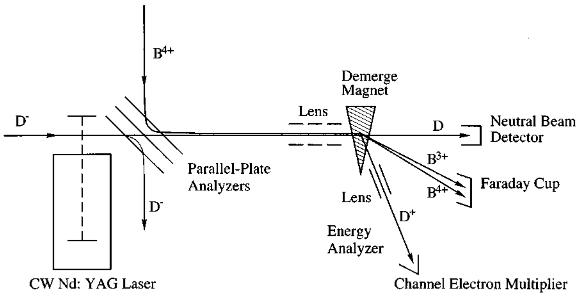

FIG. 1. A simplified schematic drawing of the ion-atom merged-beam setup.

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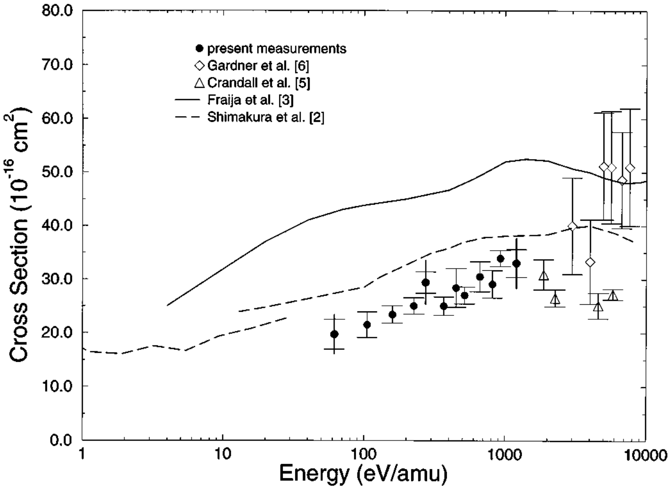

FIG. 2. A comparison of the dependence on the collision energy of experimental and theoretical total electron-capture cross sections of the B^{4+}+D system. See text for details.

is extracted from a duoplasmatron source. The obtained D beam is nearly parallel (the divergence is less than 0.15°), has a diameter of about 2 mm, and an intensity of 10–20 nA.

The B^{4+} beam is merged electrostatically with the neutral D beam. Both beams interact along a field-free region of 47 cm (see Fig. 1), after which the primary beams and the product D^+ ions are separated magnetically. The neutral beam is monitored by measuring secondary emission from a stainless steel plate, and the intensity of the B^{4+} beam is measured using a Faraday cup. The product signal D^+ ions are detected by a channel electron multiplier. The absolute electron-capture cross section is obtained from directly measurable parameters including the beam intensities, beam velocities, beam-beam signal rate, and the beam-beam overlap integral [8]. The beam velocities are calculated from the energies of the beams, which included the estimated plasma potential shifts of the two sources (see, e.g., Ref. [12]). The relative velocity (energy) is calculated from the beam energies and the relative merge angle between beams.

III. RESULTS AND DISCUSSION

In Fig. 2 the measured electron-capture cross section of the B^{4+}+D system is shown as a function of collision energy. The error bars on the experimental data indicate the statistical error at a 90% confidence level. At several energies the total uncertainty, which is a quadrature sum of the relative uncertainties and the systematic error (12%, see Ref. [15]) is also shown. Table I also lists the data and includes both relative and total errors.

As can be seen in Fig. 2, the present data show good agreement with the measurements of Crandall, Phaneuf, and Meyer [5] at 2000 eV/amu. At higher collision energies, the measurements of Gardner *et al.* [6] are larger than those of Crandall, Phaneuf, and Meyer, by almost a factor of two, but with relatively large uncertainties. Reasonably good agreement is shown between the present measurements and the semiclassical calculations of Shimakura, Suzuki, and Kimura [2], especially with respect to the energy dependence of the cross section. The calculations are still approximately 20% higher than the measurements, but are only just outside the absolute error bars. Quantum-mechanical calculations by Shimakura, Suzuki, and Kimura [2] extend the cross section to lower energies. The calculations of Fraija, Allouche, and Bacchus-Montabonel [3] are almost a factor of two larger than our measurements and seem to overestimate the cross section. The discrepancy between this theory and our experiment is not understood, but certainly the cross section is sensitive to the molecular potentials used [4], since small differences in the potential energy curves can lead to significantly different splittings, and, as a result, to large differences in the calculated cross sections. Shimakura, Suzuki, and Kimura [2] used modified valence-bond configuration interaction to calculate the pseudopotentials for the molecular orbitals, while Fraija, Allouche, and Bacchus-Montabonel [3] used *ab initio* potentials. It is not clear *a priori* which potentials are most accurate in describing the capture process, and whether the observed differences mainly arise from the (slightly) different potential energy curves used. Further theoretical investigation is needed to resolve this issue.

TABLE I. Ion-atom merged-beam cross section data for B^{4+} +D as a function of collision energy. Also listed are the relative uncertainty and total combined (relative plus systematic) uncertainty estimated at the 90% confidence level.

Collision energy (eV/amu)	Cross section (10^{-16} cm^2)	Relative uncertainty (10^{-16} cm^2)	Total uncertainty (10^{-16} cm^2)
1200	33.0	2.6	4.7
926	33.9	1.5	4.3
812	29.1	2.6	4.4
661	30.5	2.8	4.6
516	27.0	1.6	3.6
448	28.4	3.6	5.0
367	25.0	1.7	3.4
273	29.4	2.0	4.1
225	25.0	1.5	3.4
159	23.4	1.6	3.3
105	21.5	2.4	3.5
61.5	19.7	2.8	3.7

By comparing the present measurements to the predicted electron-capture cross section for the fully stripped Be^{4+} ion colliding with H, one could in principle assess the effect of the core electron on B^{4+}+H. Shimakura, Suzuki, and Kimura [2] state that at low collision energies the core-electron effect should be rather strong, because the longer interaction time causes complex multichannel and multielectron interactions. In general, collision systems with closed-core or no-core (fully stripped) ions should have lower capture cross sections than open-core systems of the same charge, because the energy splittings at the avoided crossings are somewhat wider due to the lack of strong electron mixing [2]. At high energies such effects are expected to be weak, since the collision dynamics becomes predominantly impulsive and depends mainly on the projectile charge and the collision velocity.

Several theoretical approaches to the calculation of the Be^{4+}+H cross section have been reported in the literature. The theoretical efforts of relevance at the low energies considered in this paper comprise the semiclassical atomic-orbital two-center close-coupling method [16], as well as the semiclassical molecular-orbital close-coupling method [17], the adiabatic superpromotion (or hidden-crossing) model [18], and the classical-trajectory Monte Carlo (CTMC) method [19]. Although not shown in Fig. 2, the atomic- and molecular-orbital calculations for $\mathrm{Be}^{4+}+\mathrm{H}$ are very similar to our measurements for $\mathrm{B}^{4+}+\mathrm{H}$, suggesting that if there is a clear core-electron effect it might only become noticeable at energies well below 200 eV/amu . On the other hand, the superpromotion and CTMC results indicate a significant effect (25–45 % lower cross section) even at 1 keV/amu. More theoretical work and low-energy experimental cross sections for $\mathrm{Be}^{4+}+\mathrm{H}$ are therefore needed.

IV. CONCLUSIONS

In the collision energy range of 60–1200 eV/amu, independent, absolute, total electron-capture cross sections for $\mathrm{B}^{4+}+\mathrm{H(D)}$ have been measured, using a merged-beam setup. Good agreement is observed with the measurements of Crandall, Phaneuf, and Meyer [5] at the highest energy, while reasonably good agreement is found with the calculations of Shimakura, Suzuki, and Kimura [2], in particular with respect to the energy dependence, over the entire energy range. Calculations by Fraija, Allouche, and Bacchus-Montabonel [3] are almost a factor of two larger than the measurements. Such a discrepancy may be due to the sensitivity of the cross section on the molecular potentials.

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