3.2. Collisions of Be^{q+} and B^{q+} Ions with H, H_2 and He

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1. Introduction

From the perspective of applications in fusion-energy research, the relevant heavy-particle collision processes involving Be^{q+} and B^{q+} ions are charge exchange, excitation and ionization in collisions with H, H_2 and He. The collision energy range considered is 10 - 10^6 eV per nucleon. The lower energies are relevant to modelling and diagnostics of the edge or scrape-off plasma, while the higher energies are important for diagnostics and energy-deposition in the plasma using energetic neutral beams of H or He. Collisions between Be and B impurity atoms and ions themselves are considered to occur too infrequently to play a significant role in such plasma devices. Such collisions are most often studied experimentally, by passing energetic ion beams through gaseous targets. Therefore, in the following discussion, Be or B ions will be referred to as the projectile and H, H_2 or He as the target.

The availability of data for charge exchange, excitation and ionization in collisions of Be^{q+} and B^{q+} ions with H, H_2 and He are summarized in Table 1, where "E" refers to experimental data and "T" to theoretical data. For excitation and ionization collisions, the subscripts "t" and "p" refer to target and projectile, respectively. For electron-capture collisions involving He or H_2, the subscripts "1" and "2" refer to the transfer of one or two electrons, respectively. New theoretical data which were presented at this meeting are also included in Table 1.

Semiempirical scaling relationships for heavy-particle collisions are often applied for higher-Z impurities. For example, such a formula for charge-exchange collisions [1] may be used quite reliably for impurities such as Fe or Ni in ionization stages higher than 5. This scaling formula is, however, generally not applicable to low-Z impurities such as Be and B, for which each collision system must be considered individually. One exception is the ionization of H, H_2 or He by Be^{q+} or B^{q+} ions at energies above 20 keV/amu, where scaling formulae based on the Bethe approximation [2,3] may be used with some reliability.

2. Charge Exchange

Charge-exchange (electron-capture) collisions between impurity ions and neutral H, H_2 and He are by far the most important heavy-particle processes occurring in fusion plasmas because of their relatively large cross sections at lower kinetic energies. This results from the exothermicity of such reactions involving multiply charged ions. At near-thermal energies such as those prevailing in the edge plasma, cross sections for charge exchange are very sensitive to the degree of exothermicity of a particular channel. Those which have appreciable cross sections generally leave the ion in an excited state and are exothermic by several electron volts, depending on the initial charge of the ion. Photon emissions from excited impurity ions are important for diagnostics involving the use of injected neutral beams of H or He.

The data for total and partial cross sections for electron transfer collisions of Be^{q+} and B^{q+} ions with H, H_2 and He have been recently compiled by Tawara [4] in preparation for this meeting. New coupled-state calculations were presented by Kimura [5] for Be^{q+} + H, Be^{q+} + H_2 (q=2,3,4) and B^{q+} + H, B^{q+} + H_2 (q=3,5). These are based on molecular orbitals (MO) with electron-translation factors at low energies, and the extended atomic-orbital method (AO+) at higher energies. New calculations for Be^{4+} + H and B^{5+} + H based on the "adiabatic hidden crossings" or "superpromotion" model were also presented by Krstic [6]. This method gives reliable partial cross sections for capture into a particular n shell down to 0.3 keV/amu. An intercomparison of the various theoretical methods that have been applied to the electron-capture process shows that the predicted cross sections for capture into specific states are very sensitive to the method applied, whereas the total cross sections are rather insensitive.

Be^{+} + H, Be^{+} + He:
Neither experimental nor theoretical cross-section data are available for these reactions. Since they are endothermic in all channels, the cross sections are expected to be very small for E < 1keV/amu.

Be^{2+} + H:
No experimental data are available. Theoretical perturbed-stationary-state (PSS) calculations of Wetmore et al [7] agree within 10% with the new coupled-state calculations (AO-MO) of Kimura [5], which include electron translation factors and a larger basis. The latter are recommended for the total cross section, and for capture to the 2s and 2p states. Data are needed at energies above 10 keV/amu.

Be^{3+} + H:
No experimental data are available. Molecular coupled-state calculations employing electron translation factors have been performed by Shimakura [8] for capture to the 2s, 2p, 3s, 3p, and 3d states, and for the total capture cross section. The accuracy of the total cross section is estimated to be 30-50% at energies above 25 keV/amu, and 20-30% at lower energies. The n=2 partial cross sections (dominant channels) are estimated to be accurate to 20-30% and the n=3 cross sections to 30-50%.

Be^{4+} + H:
No experimental data are available. Total and partial cross- section calculations have been performed by Fritsch and Lin [9] (AO) and by Kimura [5] (AO-MO). New low-energy calculations were presented by Krstic [6] based on the superpromotion model. In the 0.1-5 keV/amu energy range, all three calculations agree to within 5% for the total cross section, as well as for state-selective capture to the dominant channels (n=3). For the non-dominant (n=4) channels, the agreement is less satisfactory. Unitarized- distorted-wave (UDWA) calculations of Ryufuku [10] are available at energies above 10 keV/amu. The accuracy of the total and n=3 cross sections is estimated to be 10% at energies in the 0.1-5 keV/amu range, and 20% at higher energies. The accuracy of the n=4 and n=5 cross sections is estimated to be 20-50%. New low-energy total and partial cross-section data for capture from H^{*}(n=2) were presented by Krstic [6]. The accuracy of these data is unknown at the present time.

B^{+} + H:
Experimental total cross-section measurements using the ion-beam -gas-target method have

been made by Goffe et al [11] at energies between 10 and 150 keV/amu. The estimated accuracy is 10-20%. Since all channels are endothermic, the cross section is expected to decrease at lower energies. No state-selective or theoretical data have been reported.

B^{2+} + H:

Total cross-section measurements based on the ion-beam - gas-target method have been reported by Goffe et al [11], McCullough et al [12], Crandall et al [13] and by Gardner et al [14]. These data are consistent and cover the energy range from 2-200 keV/amu. No state-selective or theoretical data are available. The estimated accuracy is 10%, except at the lowest and highest energies where it is estimated to be 20%.

B^{3+} + H:

Experimental total cross-section data have been obtained over the energy range 1-200 keV/amu using the ion-beam - gas-target method by Goffe et al [11], McCullough et al [12], Crandall et al [13] and Gardner et al [14]. Molecular-orbital coupled-state calculations by Olson et al [15] and by Wetmore et al [16] agree well with the experimental data and extend down in energy to 0.3 keV/amu. The uncertainty of the data is estimated to be 20-30% in the energy range 0.3-2 keV/amu and 10-15% from 2-200 keV/amu. Partial cross sections have been calculated Kimura [5] for capture to the 2s and 2p states, with estimated accuracies comparable to those of the total cross section for 2p and somewhat larger for the 2s state.

B^{4+} + H:

Experimental data based on the ion-beam - gas-target method are available for the total cross section at energies between 2 and 200 keV/amu from Goffe et al [11], Crandall [13] and Gardner et al [14]. Calculations by Olson and Salop [17] based on the classical trajectory Monte Carlo (CTMC) method in the energy range 10-150 keV/amu are in agreement with the experimental data. The estimated accuracy of the total cross section is 10-20%. No state-selective or low-energy total cross-section data are available.

B^{5+} + H:

Both total and state-selective cross-section data are available for this reaction. Experimental total cross-section data based on the ion-beam - gas-target method have been reported by Goffe et al [11], Crandall [13] and Bendahman et al [18] over the energy range 0.2-200 keV/amu, and are in good agreement with each other. Theoretical total cross-section data of Ryufuku [10] based on the UDWA approximation, Fritsch and Lin [9] based on the AO coupled-states method, and Krstic [6] using the superpromotion model agree well with experiment. The accuracy of the total cross section is estimated to be 10% for energies in the range 0.2-200 keV/amu. Total cross-section data are needed at energies below 200 eV/amu.

In the energy ranges where they overlap, partial cross-section calculations by Fritsch and Lin [9], Ryufuku [10] and Kimura [5] agree within estimated accuracies of 10% for n=4, 20% for n=3, and 30% for n=5. For the non-dominant channels (n=2,6,7,8), the cross sections are small, and only the UDWA calculation of Ryufuku [10] at higher energies and the superpromotion model calculation of Krstic [6] at lower energies are available. Since their energy ranges do not overlap, the uncertainty is difficult to assess for these channels. New total and partial cross-section calculations were also reported by Krstic [6] for capture from H*(n=2). The accuracy of these data is unknown at the present time.

Be^{+} + H_2:

The only reported data are single-capture measurements by Sherwin [18] in the 1-3 keV/amu energy range. Their is difficult to assess.

$Be^{2+} + H_2$, $Be^{3+} + H_2$, $Be^{4+} + H_2$:
Experimental single-capture cross-section measurements of Takagi et al [19] based on the ion-beam - gas-target method are available in the 0.1-1 keV/amu energy range. Total cross sections have also been calculated for these reactions in the 0.1-9 keV/amu energy range by Kimura [5], and partial cross-section calculations are in progress. The accuracy of the total cross-section data is estimated to be 20%. Additional data would be useful at energies above 10 keV/amu.

$B^{+} + H_2$:
The only available data are single-capture cross-section measurements reported by Goffe et al [11] at energies between 10 and 150 keV/amu, to which the accuracy is estimated to be 10-20%. Additional data at lower energies would be useful.

$B^{2+} + H_2$:
Experimental data based on the ion-beam - gas-target method are available for the total single-capture cross section at energies between 0.3 and 200 keV/amu from Goffe et al [11], Crandall [13], McCullough et al [12] and by Gardner et al [14]. The data of Gardner et al appear to be low by 50%. An estimated accuracy of 20-25% is assigned to the data for this reaction. Since the cross section is unusually large for a doubly charged ion, and increases with decreasing energy, additional experimental and/or theoretical data at lower energies would be useful.

$B^{3+} + H_2$:
Total single-capture cross-section measurements have been reported by Goffe et al [11], Crandall [13], and by Gardner et al [14] over the energy range 1-200 keV/amu. New theoretical data were also presented by Kimura [5] in the energy range 0.1-10 keV/amu, which agree well with the measurements. The accuracy of the data for this reaction is estimated to be 20%. Double-capture measurements have also been reported by Gardner et al in the 1-5 keV/amu energy range. The double-capture cross section is unusually large relative to single capture in this case.

$B^{4+} + H_2$:
Total single-capture cross-section measurements have been reported by Goffe et al [11], Crandall [13], and by Gardner et al [14] over the energy range 2-200 keV/amu. The accuracy of the data for this reaction is estimated to be 20%. Double-capture measurements have also been reported by Gardner et al in the 2-5 keV/amu energy range. The double-capture cross section is negligibly small relative to single capture in this case.

$B^{5+} + H_2$:
Total single-capture cross-section measurements have been reported by Goffe et al [11] and by Crandall [13] over the energy range 5-200 keV/amu. New theoretical data were also presented by Kimura [5] in the energy range 0.1-10 keV/amu, which are consistent with these measurements. The accuracy of the data for this reaction is estimated to be 15-20%.

$Be^{+} + He$:
The only data for these reactions are angular differential total cross-section measurements by Ostgaard Olsen et al [19] in the 200-500 eV/amu energy range, and by Gay et al [20] at 56.25 keV.

Be^{2+} + He:
No experimental or theoretical cross-section data are available for this reaction.

Be^{3+} + He:
Theoretical Landau-Zener calculations have been reported by Boyd and Moiseiwitsch [21] for capture into the 2^3S, 2^3P and 2^1P states in the energy range 0.1-1000 eV/amu. No experimental data are available.

Be^{4+} + He:
Only theoretical data are available for this reaction. Total single-capture cross sections have been calculated by Olson [22] using the CTMC method, and by Suzuki et al [23] using the exponential distorted-wave approximation. These calculations are consistent with one another at energies where they overlap and cover the range 1-400 keV/amu. The accuracy is estimated to be 15-20%. Partial cross sections for single and double capture have also been reported by Martin et al [24] in the 0.25-20 keV/amu energy region.

B^{+} + He:
The only data are total cross-section measurements by Nikolaev et al [25] at energies in the 10-100 keV/amu range. Data are needed over a wider energy range.

B^{2+} + He:
Experimental single-capture data have been reported by Sherwin [18], Gardner et al [14], and by Nikolaev et al [25], covering the energy range 0.5-400 keV/amu. There is a large (order-of-magnitude) discrepancy between the data of Sherwin and those of Gardner et al at energies below 5 keV/amu. Above 40 keV/amu, the uncertainty is estimated to be 20%. There is a gap in the data between 4 and 40 keV/amu. Additional data are required at energies below 40 keV/amu.

B^{3+} + He:
Experimental total single-capture cross-section data have been reported over the energy range .04-400 keV/amu by Crandall [13], Gardner et al [14], Nikolaev et al [25], Zwalley and Cable [26] and Iwai et al [27]. Theoretical coupled-state calculations have also been reported by Shipsey et al [28] over the energy range .03-6 keV/amu. With the exception of the measurements of Gardner et al [14], these data are very consistent with one another, and an accuracy of 10-20% is estimated. Shipsey et al also reported partial cross section calculations for capture into the 2s and 2p states, whose ratio is confirmed by Matsumoto et al [29]. An accuracy of 10-20% is estimated for these partial cross sections as well. Double-capture cross-section measurements reported by Crandall [13] show an unusual energy dependence. The cross section is small relative to single capture, and likely unimportant for applications.

B^{4+} + He:
Experimental data have been reported for the total single-capture cross section by Gardner et al [14], Nikolaev et al [25] and by Iwai et al [27]. These data span the energy range 0.5-800 keV/amu, but a significant gap exists between 8 and 200 keV/amu, where further data are needed. No theoretical or partial cross-section data are available. An accuracy of 20-30% is estimated in the energy ranges 0.5-8 keV/amu, and 200-800 keV/amu.

B^{5+} + He:

Experimental data have been reported for the total single-capture cross section by by Iwai et al [27], Nikolaev et al [25] and Guffey et al [30]. Theoretical data based on the CTMC method by Olson [22] tie in well with the measurements. While these data span the energy range 0.5-800 keV/amu, a significant gap exists between 2 and 100 keV/amu, where further experimental and/or theoretical data are needed. The accuracy is estimated to be 20% at energies below 2 keV/amu and above 100 keV/amu.

4. Excitation

Data on excitation of H, H_2 and He (targets) by multicharged (projectile) ion impact are extremely limited. A small number of theoretical calculations have been reported for excitation of ground-state hydrogen atoms by bare Be and B ions; these are outlined below. No such data exist for partially-stripped Be or B ions, although a charge and energy scaling relation has been developed for multicharged ion impact on He. No data exist for excitation in collisions of Be^{q+} or B^{q+} ions with H_2. Dissociative excitation of H_2 could play an important role in fusion plasmas. Excitation of fine-structure ($\Delta n=0$) transitions in H^+ + Be^{q+} and H^+ + B^{q+} collisions can have relatively large cross sections and play an important role for partially stripped Be and B impurities.

<u>Be^{4+} + H(1s):</u>
The two-state dipole-close-coupling approximation (DCC) has been applied by Janev and Presnyakov [31] to n=1 -> n=2,3,4 excitation of H by Be^{4+} ion impact at energies ranging from 2-100 keV/amu. Fritsch [32] has recently performed extended atomic-orbital close-coupling (AO+) calculations for n=1 -> n=2 excitation of H by Be^{4+} impact at energies ranging from 6 to 50 keV/amu. New theoretical data in the 1-30 keV/amu energy range based on the superpromotion model were also presented by Krstic [6]. The latter results are recommended with an estimated accuracy of a factor of 2. These data are consistent within a factor of 3 or better with the AO+ calculations, and to within an order of magnitude with the DCC calculation. Data are needed for for excitation from n=1 -> n=3,4 and n=2 -> n=3,4.

<u>B^{5+} + H(1s):</u>
The unitarized distorted-wave approximation (UDWA) has been applied by Ryufuku [33] to the total excitation cross section (summed over excitations to all n). New theoretical data in the 1-30 keV/amu energy range based on the superpromotion model were also presented by Krstic [6] for n=1 -> n=2 excitation. These latter data are recommended with an estimated factor-of-two accuracy. Again, data are needed for for excitation from n=1 -> n=3,4 and n=2 -> n=3,4.

<u>Be^{q+} + He, B^{q+} + He:</u>
A charge-scaling relation has been derived from experimental data by Reyman et al [34] for excitation of a He target by a variety of multicharged ion projectiles with charges ranging from 6 to 44 and energies from 120 to 1000 keV/amu. This scaling relation is estimated to be reliable in predicting the He excitation cross sections to within a factor of 2 at 100 keV/amu, and better at higher energies. Experimental and theoretical cross-section data for projectile 2s-2p excitation of Be^+ in collisions with He have also been reported by Andersen et al [35] and Nielsen et al [36] respectively, over the energy range .05-40 keV/amu. Such data may be useful for diagnostic purposes.

5. Ionization

The only experimental data for ionization of H, H_2 or He by Be^{q+} or B^{q+} impact are measurements by Haugen et al [37] for single ionization of He by B^{3+}, B^{4+} and B^{5+} at energies ranging from 190 to 2310 keV/amu. These have an estimated accuracy of 20%. Andersen [38] has also reported double ionization cross sections for these same reactants and energy range, and has investigated their scalings with ionic charge.

The CTMC method has been employed by Olson [39] and by Pfeifer and Olson [40] to Be^{4+} + He and B^{5+} + He collisions at energies in the 100-500 keV/amu range. New theoretical data were also presented by Krstic [6] based on the superpromotion model for ionization of H(n=1) and H(n=2) by Be^{4+} and B^{5+} impact at energies ranging from 0.4-30 keV/amu. The accuracy of these data are difficult to assess. Nikolaev et al [41] have also reported calculations based on the Bethe-Born approximation for Be^{2+} + H and Be^{2+} + He collisions at energies ranging from 6 keV/amu to 25 Mev/amu. Goffe et al [42] have also reported projectile ionization or stripping cross-section measurements for B^{+} and B^{2+} colliding with H and H_2 at energies in the 10-200 keV/amu range.

In general, for ionization of H, H_2 or He by Be^{q+} or B^{q+} ions at energies above 50 keV/amu, where ionization dominates electron capture, scaling formulae of Gillespie based on the Bethe approximation [2,3] may be used to predict the target single- ionization cross section with an estimated accuracy of 10-30%. At lower energies, where the ionization cross sections become very small, and the capture process dominates, theoretical methods and scaling laws are generally unreliable. Tabata et al [43] have modified the Gillespie scaling relations to better represent what low-energy data are presently available, but experimental data are needed for all these collision systems at energies $E/q < 50$ keV/amu to establish the low-energy behavior of the ionization cross sections. These and additional data at higher energies are needed to provide important tests of such scaling relations.

6. Two-Electron Processes

For collisions involving H_2 and He, two-electron collision processes must also be considered. Examples are double electron capture, transfer-ionization at lower energies, and double ionization at higher energies. Cross sections for these processes are generally an order of magnitude smaller than those for single-electron processes. Relatively less attention has been devoted to such processes.

6. References

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Table 1. Availability of Data for Collisions of Be^{q+} and B^{q+} Ions with H, H_2 and He

Target (t)	H					H_2					He				
Projectile (p)	TC	SSC	ANG	EX	ION	TC	SSC	ANG	EX	ION	TC	SSC	ANG	EX	ION
Be^+						E_1							T_1 E_1	T_p E_p	
Be^{2+}	T	T			T_t	T_1 E_1	T_1								T_t
Be^{3+}	T	T				E_1	T_1					T_1			
Be^{4+}	T	T		T_t	T_t	E_1	T_1				T_1				T_t
B^+	E				E_p	E_1					E_1				
B^{2+}	E				E_p	E_1				E_p	E_1 E_2				
B^{3+}	T E	T				E_1 E_2	T_1				T_1 E_1 E_2	T_1 E_1			E_t
B^{4+}	T E					E_1 E_2					E_1				E_t
B^{5+}	T E	T	T_t	T_t	T_t	T_1 E_1					T_1 E_1 E_2				T_t E_t

TC = total electron capture (summed over final states)
SSC = state-selective electron capture
ANG = data on angular distribution of products of electron-capture collisions
EX = excitation of projectile (p) or target (t)
ION = ionization of projectile (p) or target (t)
E = experimental data
T = theoretical data
1,2 = single or double electron capture