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Theoretical study of Na excitation and ionization in $H^+ + Na$ collisions

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Na excitation and ionization cross sections in $H^+ + Na$ collisions are determined at impact energies 0.7–50 keV within the semiclassical close-coupling method with atomic-orbital basis sets including pseudostates. Calculated $Na(3s \rightarrow 3p)$ excitation cross sections and the $3p$ alignment show structures which agree very well with available experimental data. While a structure at 3 keV is predominantly caused by interaction between capture and excitation channels, interaction between excitation and ionization channels leads to a shoulder in the calculated $3p$ excitation cross section at higher energies and a correlated distinct dip in the predicted ionization cross section.

In this paper we report on a theoretical investigation of electron excitation and ionization in $H^+ + Na$ collisions at impact energies 0.7–50 keV. The aim of this investigation is mainly to clarify the following points. (i) A number of measurements,[1–4] including very recent ones, on $Na(3s \rightarrow 3p)$ excitation in $H^+ + Na(3s)$ collisions, while agreeing qualitatively on the energy dependence of the excitation cross section, disagree on its absolute magnitude. (ii) The measured $3p$ excitation cross sections show a slight dip,[3,4] or at least some plateaulike structure,[1,2] roughly around the energy where the transfer cross section peaks. This structure is either not seen in the results of previously published theoretical investigations[5,6] or appears to be stronger[7] than in the experimental data. (iii) The measured $3p$ alignment[3] shows some structure which has not yet been reproduced in calculations. (iv) As will become clear below, an assessment of ionization in $H^+ + Na$ collisions is a by-product of this investigation. It is reported here for comparison with future experiments.

An earlier, much more disturbing situation of mutually disagreeing experimental and theoretical *transfer* cross sections for $H^+ + Na$ collisions has been addressed with an atomic-orbital (AO) expansion calculation.[8] There is now overwhelming experimental[4,9,10] and theoretical[5–7] evidence in support of the results reported in Ref. 8. There is no doubt that an AO expansion calculation for electron excitation should be as reliable as the similar calculation for electron capture, provided that the important physical channels are included in the calculation. Moreover, with present-day methods and computer codes, the determination of cross sections for a fairly strong channel in a quasi-one-electron system is a straightforward task.

Therefore, in this investigation, as in the earlier one on electron transfer,[8] the $H^+ + Na$ collision system is described as a quasi-one-electron system in which the Na^+ core is represented by a non-Coulombic potential. The calculations are done within the semiclassical close-coupling method, with AO's and some pseudostates representing the motion of the electron during the collision.[11] Since electron transfer and electron excitation constitute strong channels in the $H^+ + Na$ collision system at intermediate energies, they have to be included jointly in the calculations no matter whether one is interested in the final transfer or excitation cross sections; indeed, if the calculations reported earlier[8] are extended to larger impact parameters they already yield fairly reliable $3p$ excitation cross sections. Still, the model calculations reported here differ from those for the transfer channels[8] in two aspects.

(a) *The potential:* It has been noted before[8] that the calculated transfer cross sections for $H^+ + Na$ collisions are largely insensitive to the choice of the Na^+ core potential. When extracting $3p$ excitation cross sections, however, it turns out that results derived with the model potential by Peach[12] and with the pseudopotential by Bardsley[13] (the latter has been used in Ref. 8) differ by as much as 15%. Since, in contrast to a pseudopotential, a model potential leads to the correct nodal structure of the wave function it was decided to use it for the present calculations.

(b) *The AO basis:* We have chosen to include into the AO basis set not only the $n=1-3$ capture and the $3p$ and $3d$ excitation channels as in Ref. 8, but also the $4s$, $4p$, and $4d$ excitation channels so that, for comparison with experiment, feeding of the $3p \rightarrow 3s$ decay by cascades from higher excitation channels can be assessed better than before. Moreover, since details of the excitation cross section, like the occurrence and the shape of the dip seen in experiment, can well be influenced by competition of excitation with capture *and* ionization channels,[14] the latter have been included by the same set of pseudostates, which was used for that purpose already for $H^+ + H$ collisions.[14] Therefore, as in earlier work,[14] the AO basis is taken to consist, at the H center, of the $n=1-3$ H orbitals and some $nl(Z)$ hydrogenic orbitals with charge number Z $[nl(Z)=1s(0.65,1.56,2.44),2p(0.667,1.8,2.9,4.5)]$ and, at the Na center, of the same orbitals as before (with the omission of $3d$ H orbitals) plus $1s(10.5)$ and $4d(1.01)$ hydrogenic orbitals as well as $2s(8.6)$, $2p(3.4)$, and $3d(0.34)$ Slater orbitals. Thus, including all m substates, the basis consists of 49 states. The calculation starts from linear combinations of those orbitals, which result from diagonalizations of the atomic Hamiltonians within the given orbitals. The linear combinations with the lowest energies constitute good representations of the lowest bound states of the respective atoms; those with positive energies are taken as representations of the continua of target and projectile.

The linear combinations with the five highest energies were left out of the calculation in order to speed up the numerical integration of the coupled equations.

The calculated cross sections for population of Na($3p$) states with and without cascading contributions[15] from higher orbitals, for population of $3d$ states with cascading contributions, and for ionization are displayed in Fig. 1. The results for $3p$ population including cascade contributions show a maximum at about 15 keV in agreement with the maximum in the data by Howald *et al.*[1] with an additional broad shoulder on the high-energy side of the maximum where experimental data are sparse. The plateau-like structure at 2–4 keV agrees nicely with similar structures in the respective results measured by Lavrov and Lomsadze,[2] Jitschin *et al.*,[3] and Aumayr, Lakits, and Winter.[4] In absolute magnitude, the calculated results agree very well with the data by Lavrov and Lomsadze at all energies and still reasonably well with the other data except for the data by Jitschin *et al.*[3] which are consistently higher by about a factor of 1.6.

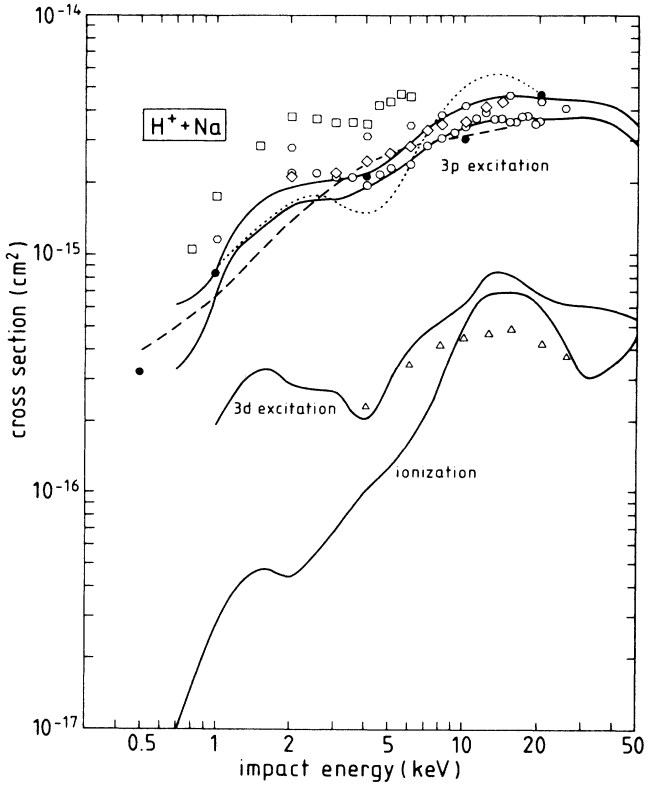

FIG. 1. Cross sections for Na($3p$) and Na($3d$) excitation and ionization in $H^+ + Na$ collisions. Theoretical Na($3p$) excitation cross sections. This work: upper two full curves; the uppermost curve includes the population of $3p$ states from the decay of higher excited states and as such indicates a $3p \rightarrow 3s$ line emission cross section. AO calculations by Shingal *et al.* (Ref. 6) (filled circles) and by Ermolaev (Ref. 7) (dotted line); MO calculation by Allan (Ref. 5) (broken line). Experimental data, indicated by open symbols, are by Howald *et al.* (Ref. 1, hexagons), Lavrov and Lomsadze (Ref. 2, diamonds), Jitschin *et al.* (Ref. 3, squares), and by Aumayr *et al.* (Ref. 4, circles). The lowest full line indicates the ionization cross section calculated in this work. The curve labeled "$3d$ excitation" indicates calculated cross sections including cascade contributions. Experimental (Ref. 16) $3d$ excitation cross sections are indicated by open triangles.

Results for $3p$ excitation (without cascading contributions) from the other calculations also follow roughly the trend of the experimental data but seem to miss some of the details of the latter. The cross sections from the AO calculations by Shingal *et al.*[6] are too widely spaced in energy to make predictions about the plateau around 3 keV, and seem to get a maximum larger in magnitude than would be consistent with experiment (including cascades). The AO results by Ermolaev[7] show distinctively more structure than the one presented here. On the other hand, the results from the molecular-orbital (MO) calculation by Allan (which are published[3] as a smooth line) do not show any plateau. Some of the difference between results from various model calculations may be attributed to the fact that different potentials have been used in the calculations. The major portion of that difference, however, is probably due to the choice of different basis sets for the calculations. In particular, in the MO calculation the most important of the $n=2$–3 H and $n=3$, $4s$,$4p$ Na orbitals (though not all of them) are included but not any continuum states, while in the other two AO calculations some pseudostates are included but without apparent consideration for their representation of the projectile and target continua.

The calculated cross sections for excitation into individual higher excited states show also some structure. Among those channels, the $3d$ excitation channel is the strongest, and the calculated cross section for its population (including contributions from cascades) is compared with the data by Anderson, Allen, Lin, and Miers[16] in Fig. 1. Clearly, the agreement for this channel is by far less satisfactory than for $3p$ excitation. The calculated population of $4s$, $4p$, and $4d$ channels turn out to be, among the $n=4$ excitation channels, of similar magnitude. Details about these smaller excitation channels are available from the author upon request.

In Fig. 2, the calculated alignment[17] A for the excited $3p$ Na states (with m-substate cross sections σ_1 and σ_0) is shown:

$$A=(\sigma_1-\sigma_0)/(2\sigma_1+\sigma_0) \ .$$

The rich structure in the $3p$ alignment is another indication of the strong competition (or interaction) in the course of the collision between a number of final states. The structure between 1.3- and 7-keV impact energy agrees very well with experimental data,[3] which again show that discrepancies for $3p$ excitation between theory and those data (cf. Fig. 1) are likely to be merely due to a normalization problem in that work. The MO curve published[3] together with those experimental data is less structured than the present curve.

We note that the calculated alignment shown in Fig. 2 does not contain cascading contributions. These contributions are expected to be small and may be evaluated efficiently with expressions which will become available soon.[18]

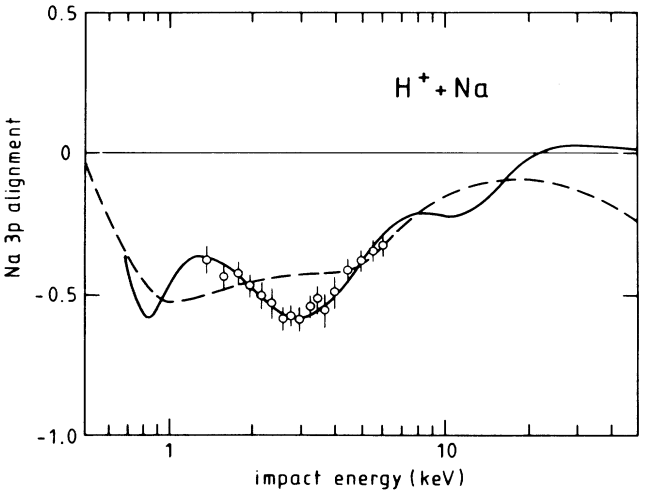

FIG. 2. Na($3p$) alignment in collisionally induced Na($3s \rightarrow 3p$) excitation. The full curve indicates results of this work, and the broken line, the results of the MO calculation shown in Ref. 3. Experimental data are also by Jitschin *et al.* (Ref. 3).

The calculated ionization cross sections are also displayed in Fig. 1. A striking feature of these cross sections is the maximum at about 15 keV which, at higher energies, is followed by a dip and another rise. Since the dip in ionization cross sections at about 30 keV is correlated with a shoulder in the $3p$ excitation cross section, this structure again suggests strong interaction between excitation and ionization channels. The small undulation at about 2 keV may be of little relevance since at very low energies the extraction of ionization cross sections from two-center expansions is known[19] to become less valid. At higher energies, however, there is sufficient evidence[14,19,20] to believe that the calculated ionization cross sections are reliable. In passing, we note that the calculated ionization cross sections are dominated by contributions from orbitals traveling with the projectile. Although it is doubtful whether a realistic momentum distribution of electrons could be extracted from the calculations we take this observation as an indication that the ionization cross sections are due to capture to the continuum rather than to direct ionization, at least over the energy range considered here.

In conclusion, a large number of interacting atomic states in both projectile and target, in the close-coupling study presented here, leads to structures in the $3p$ Na excitation channel, not only in its alignment but also in the excitation cross sections themselves. While there is quantitative agreement with the data[2] of Lavrov and Lomsadze for the excitation cross section and with the data[3] of Jitschin *et al.* for $3p$ alignment, there is at least qualitative agreement with other measurements. More data would be needed at lower and higher energies for comparison with the calculations, particularly for $3p$ alignment and for $3d$ excitation. It would be interesting to see whether the structures in the calculated ionization cross section occur also in experiment.

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