n-Selective Single Capture Following Xe^{18+} And Xe^{54+} Impact On Na(3s) And Na*(3p)

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Abstract. State selective single charge exchange n-level cross sections are calculated for collisions of Xe18+ and Xe54+ ions with Na(3s) and Na*(3p) over the energy range of 0.1 to 10.0 keV/amu. The CTMC method is used which includes all two-body interactions. Experimental state-selective cross sections and their corresponding transverse momentum spectra for Xe18+ are found to be in reasonable accord with the calculations.

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INTRODUCTION

The planned construction of a large, international, high temperature tokamak fusion reactor (ITER) in Cadarache, France [1] has renewed the interest in studying multiply-charged ion electron capture collisions. Starting in the 1970s, the tokamak fusion reactor program stimulated the studies of charge exchange processes involving collisions of multiply charged ions of C, N and O with atomic hydrogen (see [2] for a review). The collision energies of interest were in the range 1-80 keV/amu. These studies were prompted by the use of the photon emission cascade following the charge exchange process to estimate the impurity ion concentrations, the plasma temperature and its rotation.

Charge exchange processes between heavy rare gases and multiply charged projectiles are expected to play a major role in the new, large ITER reactor. In order to extract the heat from the reactor, it is proposed that charge exchange collisions in the scrape off layer and divertor will give rise to photon emission that will uniformly heat the plasma facing walls, thereby removing the possibility of the hot plasma touching the wall and causing burn-through. Heavy rare gas ions will be used as the charge exchange medium that interacts with the H (D) atoms.

Although it is well known that the H*(n=2) target provides a high fraction of the photon flux in these collisions, it has been experimentally infeasible up to now to provide experimental cross sections to test theoretical predictions. However, ground state alkali atoms have very similar cross sections due to their nearness in ionization potentials and provide substitutes that can be experimentally explored. The KVI group has recently succeeded in obtaining state-selective data for Xe18+ + Na(3s) collisions using the MOTRIMS (Magneto Optical Trap Recoil Ion Momentum Spectroscopy) method [3]. The same group has already optically pumped Na(3s) to obtain Na*(3p) targets together with He2+ and C4+ projectiles in the past [4-5] .

In this work, we use the 3-body CTMC method to obtain state selective electron capture data for the reactions:

$$\begin{aligned} Xe^{q+} + Na(3s) &\rightarrow Xe^{(q-1)+}(n) + Na^{+}, \\ Xe^{q+} + Na^{*}(3p) &\rightarrow Xe^{(q-1)+}(n) + Na^{+}. \end{aligned} \quad (1)$$

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The projectiles under study will be Xe18+ and Xe54+. The Na*(3p) target is included in our study to provide guidance for future experimental studies. The energy range investigated is 0.1 – 10 keV/amu, termed intermediate since the collision speeds surround those of the target electron which corresponds to 9.4 keV/amu for Na(3s) and 5.6 keV/u for Na*(3p).

THEORETICAL METHOD

The classical trajectory Monte-Carlo (CTMC) method has been used to calculate cross sections for single electron capture [6]. Hamilton's equations were solved for a mutually interacting three-body system. The center-of-mass of the Na target is frozen at the beginning of each simulation. The active electron evolves under the central potential model developed by Green et al. from Hartree-Fock calculations [7], and later generalized by Garvey et al. [8]. The CTMC method directly includes the ionization channel and is not limited by basis set size for the prediction of capture to very high-lying excited states. The Na(3s) and Na*(3p) states are distinguished through their respective ionization potentials and the classical angular momentum restriction $l^2<1$, and $1<l^2<4$ respectively [9].

Since the electron tends to be captured to high n-values with minimal contributions from the s-, p-, and d-states, quantum defects play a minor role and the orbital energies for the captured electron are similar to those obtained with bare projectiles. We then represent the electron-projectile interaction by a Coulomb potential of charge 18+ and 54+ respectively.

RESULTS

In Figs. 1 and 2 are presented the n-selective capture cross sections for Na(3s) and Na(3p) targets as a function of collision energy for the Xe18+ and Xe54+ systems, respectively. We note that at 1 keV/amu the total charge exchange cross sections (not shown here) for both targets under consideration scale linearly with the projectile charge as previously predicted [10]. Furthermore, the Na*(3p) total charge exchange cross sections are approximately a factor of three larger than those for the ground state. One can see that the capture process is sharply peaked in n-value at the lowest energy leading to large cross sections for only a few n-values. However, at the highest energy the n-distribution is considerably broadened due to strong mixing of the capture channels in the increasingly important small impact parameter collisions.

The theoretical cross sections presented for Xe18+ on Na(3s), Fig. 1, can be compared to experimental data obtained by the KVI group. The measurements were obtained using the newly developed MOTRIMS method [3]. In Fig. 3 are shown the data over the experimental energy range. Overall, there is good agreement between theory and experiment, indicating that theory is able to represent these strong perturbation collisions.

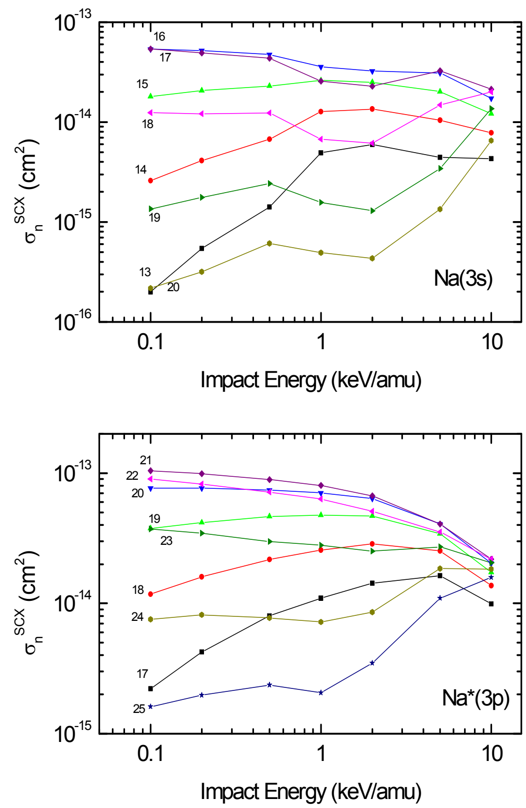

FIGURE 1. n-state selective capture cross sections for Na(3s) and Na*(3p) targets as a function of collision energy for Xe^{18+}. The final n-levels are labeled next to each curve.

A more strenuous test of theory is to compare the n-level cross sections differential in their transverse momenta. By so doing, we are testing the impact parameter dependence of the n-level transition probabilities since the transverse momentum magnitude is inversely proportional to impact parameter. In Fig. 4 are shown the transverse momentum comparisons for the n = 14, 16 and 18 levels in 2.23 keV/amu collisions of Xe18+ on Na(3s).

The data collection and analyses are described in the Ph.D. thesis of V. G. Hasan [11]. Theory reproduces the overall trends in the data. As expected, the lower n-values are formed in the hard collision, low impact parameter region, resulting in large transverse momentum. However, there are systematic differences. The main one is that theory tends to overestimate the transverse momentum peaks. From this, one can infer that theory is underestimating the range of the collisions, or overestimating the strength of the repulsive Coulomb interaction during the collision. We must also mention that in Fig. 3 and 4 we have normalized the experimental data to our cross sections in the peak region because the experimental data are relative, not absolute in magnitude.

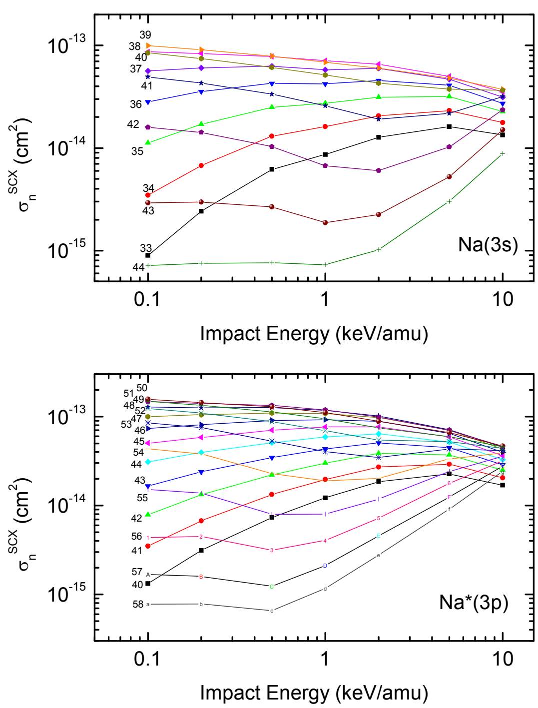

FIGURE 2. n-state selective capture cross sections for Na(3s) and Na*(3p) targets as a function of collision energy for Xe^{54+}.

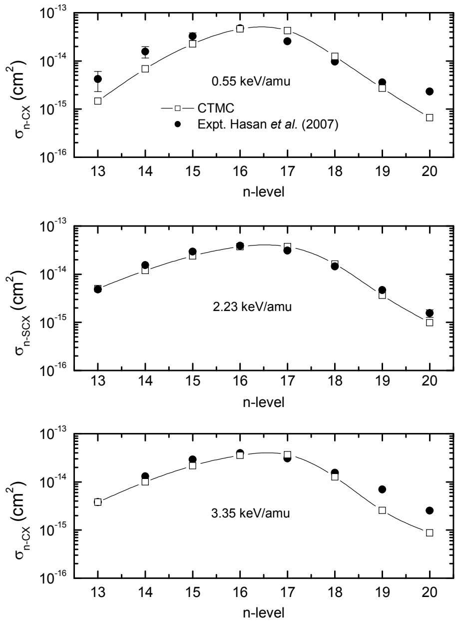

FIGURE 3. n-sate selective capture cross sections for 0.55 keV/amu, 2.23 keV/amu and 3.35 keV/amu Xe18+ collisions on Na(3s). The experimental data shown are from ref. [3].

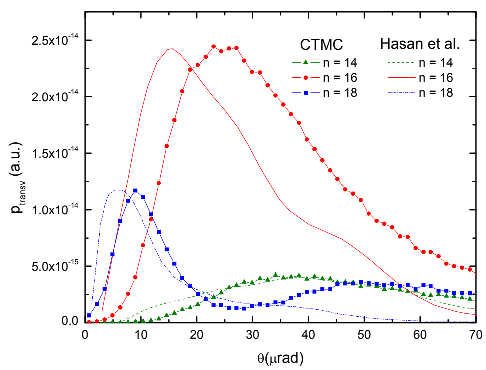

FIGURE 4. Recoil ion transverse momentum distribution at 2.23 keV/amu Xe18+ collisions on Na(3s) target (capture to n=14, 16 and 18). The experimental data shown are from Hasan (ref.[11]).

CONCLUSIONS

In this work we have studied state selective charge exchange processes for collisions of Xe18+ and Xe54+ ions with Na(3s) and Na*(3p) over the energy range of 0.1 to 10.0 keV/amu. As expected, the calculated capture cross sections from Na*(3p) are larger than those from Na(3s) and they populate larger n-values of the projectile at the same collision energy.

We have compared our theoretical predictions for the n-state selective capture cross sections and their corresponding transverse momentum spectra with available experimental data for Xe18+ +Na(3s) from the KVI group. Within the impact energy range experimentally explored, we found that our calculations are in reasonable accord with the data. These results show that the CTMC method provides a fast and confident platform for these studies.

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