Production Of $1s2s2p\,^4P$ States By Transfer-Loss Cascades In O^{5+} Collisions With He And H_2 Targets

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Single differential cross-sections for transfer-loss (TL) leading to the production of $O^{5+}(1s2s\,^3S)nl\,^4L$ states were computed for 0.2-1.2 MeV/u collisions of $O^{5+}(1s^22s)$ ions with He and H_2 targets. At these collision energies, 1s loss is significant and electron transfer to $n = 3-4$ levels is dominant. Furthermore, due to spin conservation, quartet states can only be populated by TL. Within the independent particle model, the probability of 1s electron loss from $O^{5+}(1s^22s)$ projectiles was calculated using the semi-classical approach, while the probability for electron transfer to the $O^{5+}(1s2s\,^3S)nl\,^4L$ states ($n \geq 2$) was computed using the continuum distorted wave (CDW) approximation. The majority of states with $n > 2$, can be assumed to have sufficient time to eventually decay with an almost 100% probability to the long-living metastable $1s2s2p\,^4P$ level via a much faster sequence of electric dipole transitions, thus establishing an upper limit to such cascade contributions. The inclusion of this cascade feeding is found to lead to a strong enhancement in the production of the $1s2s2p\,^4P$ states, particularly for collisions with the H_2 target, thus reducing dramatically the existing two-order of magnitude discrepancy between older TL calculations (for $n = 2$ only) and existing zero-degree Auger projectile electron spectroscopy measurements.

THE $1s2s2p\,^4P$ TRANSFER-LOSS PUZZLE

In 1989, Zouros *et al.* [1] showed that the $1s \rightarrow 2p$ projectile excitation cross section for Li-like F^{6+} and O^{5+} ions in collisions with H_2 and He (see Figs. 1-2) was found to increase when the projectile velocity V_p was such that $\frac{1}{2}\,m\,V_p^2 \gtrsim \Delta E$, where ΔE is the projectile $1s \rightarrow 2p$ excitation energy and m the mass of the electron. This enhancement of the projectile excitation cross section on passing the electron impact excitation threshold ΔE was interpreted as being due to the onset of direct projectile-electron–target-electron interactions in a process named electron-electron excitation (eeE) [1]. In reverse kinematics, the quasi-free target electrons as seen by the ion from the projectile frame, forms an "electron beam" that can excite the projectile electrons once its impact kinetic energy is larger than ΔE. This threshold, however, is partially diffused by the rather broad electron momentum distribution due to its orbital motion around the target. Today, this process is well understood within the electron scattering model [2–5] and the Born approximation [6, 7] and is found to be important in excitation [1, 7–9] and ionization [10–13] processes in ion-atom collisions [14–16]. It is particularly prevalent in ion collisions with low-Z targets, where competition from excitation due to the target-nucleus charge is relatively smaller [16].

The eeE results of Ref. [1] referred to the production of a particular state, the $1s2s2p\,^4P$, for which other competing target-nucleus excitation processes are forbidden due to spin selection rules, thus making this state uniquely accessible by the eeE process: :

$$O^{5+}(1s^22s) + e^- \rightarrow O^{5+}(1s2s2p\,^4P) + e^- \qquad (eeE) \quad (1)$$

However, below the electron impact excitation threshold ΔE, an increase in the excitation cross section of the $1s2s2p\,^4P$ state was also observed [17] in collisions of O^{5+}+He (see Fig. 2), having an energy dependence reminiscent of capture. Capture is maximized when the projectile velocity matches the velocity of the electron to be captured and drops rapidly with increasing collision energy. The production of the $1s2s2p\,^4P$ state, below ~16 MeV, showed a similar behavior which Stolterfoht *et al.* [17] attributed to the two-electron process named transfer-loss (TL). TL requires the transfer of a target electron to the projectile ion with the simultaneous loss of a projectile electron, thus leaving the projectile in a doubly-excited three-electron state. In particular, for the production of $1s2s2p\,^4P$ by TL we study the process:

$$O^{5+}(1s^22s) + X \;\rightarrow\; O^{5+}(1s2s2p\,^4P) + X^+ + e^- \quad (2)$$

due to the two independent one-electron transitions:

1s loss:
$$O^{5+}(1s^22s) \;\rightarrow\; O^{6+}(1s2s\,^3S) + e^- \quad (3)$$

2p transfer:
$$O^{6+}(1s2s\,^3S) + X \;\rightarrow\; O^{5+}(1s2s2p\,^4P) + X^+ \quad (4)$$

where X represents the target. Eqs. 3-4 seem to suggest a time-ordering of the two transitions, but in the calculations we consider them as independent events. The energy dependence of $1s2s2p\,^4P$ is shown in Figs. 1 and 2. The data refer to existing high resolution electron spectroscopy measurements of the Auger decay of the $1s2s2p\,^4P$ state observed at zero-degrees to the beam direction for O^{5+} in collisions with H_2 [1, 9, 18] and He targets [1, 9, 17, 18]. Also shown for comparison in Fig. 1 (open squares) are the 1989 results of a coupled-channel TL calculation performed by R. Shingal (shown in Fig. 1c

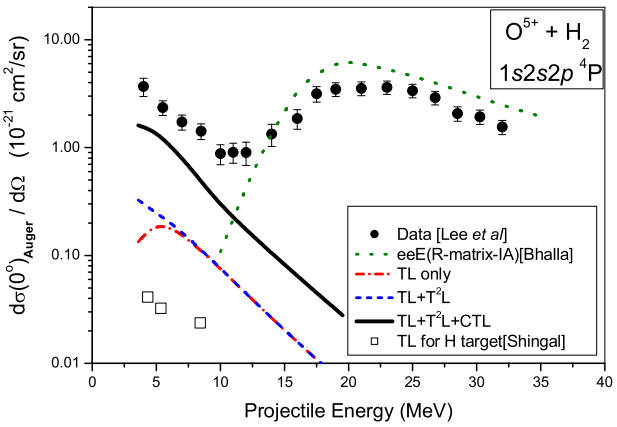

FIG. 1: (Color online). Zero-degree differential Auger projectile cross sections for producing $1s2s2p\,^4P$ states in O^{5+}+H_2 collisions. The experimental data (black circles) have been taken from Refs. [1, 9, 18]. The eeE calculation within the impulse approximation (IA) is by C.P. Bhalla [9]. The 3 open squares are from the coupled-channel calculation of R. Shingal for the O^{5+}+H system [1]. Our own TL calculations are also shown, including contributions from TL to the 2p orbital only (TL only) and upper limit estimates (see text) from double-transfer–loss (T^2L) and TL fed by cascades (CTL).

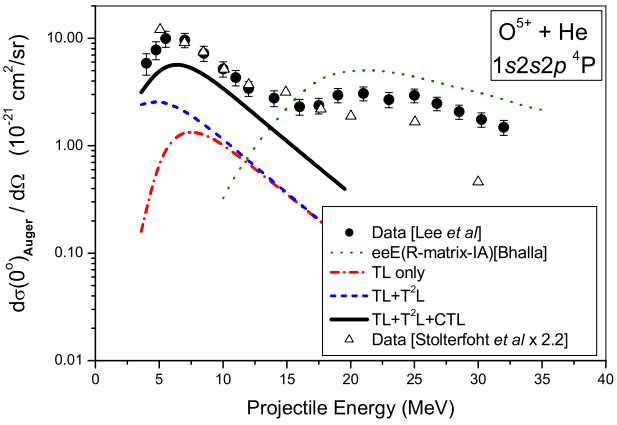

FIG. 2: (Color online). Same as Fig. 1, but for He. The open triangles refer to the data of Stolterfoht *et al* [17] converted to differential Auger cross sections and scaled by 2.2.

of Ref. [1] as a private communication) for O^{5+}+H. What was particularly puzzling at the time was that this quite sophisticated TL calculation was almost two orders of magnitude smaller than measurement. This puzzle remained uninvestigated over the next 10 years.

RECENT TL CALCULATIONS

Recently, new TL calculations were performed in the independent particle approximation (IPA) by Sulik *et al.* [19] for both H_2 and He targets using exclusive [20] unitarized [21] impact parameter b-dependent probabilities, $P(b)$. Electron transfer probabilities were computed using the continuum distorted wave (CDW) approach [22], while $1s$ loss (projectile ionization) probabilities were calculated using a semiclassical approximation (SCA) code [23] for the production of an uncoupled determinant state $|(1s2s2p_m)>$:

$$P_{TL}^{2p_m}(b) = P_T^{2p_m}(b)\cdot P_L(b) \quad (5)$$

with

$$P_T^{2p_m}(b) = P(b)[X(1s)\rightarrow O^{5+}(2p_m)]\cdot \{1-P(b)[X(1s)\rightarrow O^{5+}(\text{any shell})]\} \quad (6)$$

$$P_L(b) = P(b)[O^{5+}(1s)\rightarrow O^{6+}(\text{continuum})]\cdot \{1-P(b)[O^{5+}(1s)\rightarrow(\text{any state})]\}\cdot \{1-P(b)[O^{5+}(2s)\rightarrow(\text{any state})]\} \quad (7)$$

where X represents the He or H targets. To closer simulate the molecular H_2 target used in the experiments, the CDW and SCA calculations were performed for an effective H atom (with $Z_t^* = 1.062$) [24] including an averaging over all the orientations of the H_2 molecular axis. For the capture probability, $P_T^{2p_m}$, the term in large curly brackets represents the exclusive probability [20] that there is no other capture allowed from the other X 1s electron to the oxygen ion. In this work "any shell" represents an additional capture to oxygen. Such a capture would necessarily lead to a different ionic state with different configuration and energy and therefore to a different Auger transition which must be explicitly excluded. For the loss probability, P_L, the first term is the single ionization probability of the oxygen 1s shell, while the second and third terms represent the probabilities that the other 1s and 2s electrons of oxygen must remain untouched for the same reason as in the transfer process above. For the "any state" probabilities, the excitation from the ground state of O^{5+} into a set of excited and continuum states was considered. Finally, the uncoupled TL probabilities were then coupled together to obtain the probabilities for the specific determinant state $|(1s2s2p_m)\,^4P>$, which upon integrating over the impact parameter gave the state-selected cross section. Auger yields, and anisotropic electron emission due to alignment effects were also taken into account in calculating the theoretical zero-degree Auger emission cross section for the $1s2s2p\,^4P$ line.

Furthermore, in an attempt to investigate other possible scenarios which might further enhance the production of the $1s2s2p\,^4P$ states, the process of *double*-transfer-loss (T^2L) involving a double capture to $n>2$ levels accompanied with a $1s$ loss and followed by LXY Auger transitions was also included since it was noticed that the calculated probabilities for electron capture to $n>2$ shells were much larger than for those to the $n=2$ shell (see Figs. 3-4). However, since the various branching ratios

between the LXY Auger transitions and other competing processes were not known, and assuming that the LXY Auger transition is the dominant channel, the sum of the TL+T^2L components can be used as an *upper limit*, with the TL alone representing the calculated lower limit for the sum of the two processes. It was clearly demonstrated that the calculated T^2L contribution is much less important for the H_2 molecule than for the He atom (see Figs. 1 and 2 dashed lines).

In the above calculations of Sulik *et al.* [19], the projectile-energy dependence of the data was well reproduced for both collision systems. However, the calculated cross-sections were more than a factor of 2 too small for He and still much smaller for H_2. For the He target, the difference between the measured and calculated cross-sections was traced to the CDW capture calculations since the calculated electron loss cross-sections alone were in very good agreement with experiments [24]. For H_2, the TL calculations also seemed to be consistent with the low cross section results of R. Shingal already mentioned. The main reason for the low TL cross-sections for the hydrogen target lay in the fact that the CDW electron transfer probabilities for hydrogen were more than one order of magnitude smaller than for helium.

NEW TL CALCULATIONS: INCLUSION OF CASCADE CONTRIBUTIONS

Here, we present new improved TL calculations, along the previous lines of Ref. [19]. Small improvements include a CDW capture recalculation using the slightly larger effective $Z_t^* = 1.195$, rather than $Z_t^* = 1.062$ used previously for H_2. The justification for this change is based on the recent findings of Galassi *et al.* [25] that $Z_t^* = 1.195$ gives a better account of the initial state momentum distribution (and, in turn, the Compton profile) of the hydrogen molecule. Even double differential cross sections were found to be accurately described by applying such wave functions [24]. Using $Z_t^* = 1.195$, we obtained on average an increase in the capture probabilities from H by a factor of 1.7, closing the previously observed large capture difference between He and H target. A slightly different effective projectile charge of $Z_p^* = 6.8$ $(= 8-0.85-0.35)$ was also used to account for the partial screening by the 2 electrons in the $O^{6+}(1s2s)$ configuration. Finally, the angular emission probability was recomputed within the *intermediate* coupling scheme more appropriate for the case of the metastable $1s2s2p\,^4P$ state [26]. The newly computed angular distribution for electron emission was found to be rather close to isotropic. Accordingly, the zero-degree electron emission cross sections are smaller than their previously calculated values within the LS-coupling scheme which favored emission from the $2p_0$ sublevel for zero-degree observation.

Apart from these slight improvements that resulted in rather moderate changes in the new TL calculation, a new and very important point was also considered. As already pointed out above, the CDW calculations brought out the fact that capture to $n = 2-4$ is dominant at these collision velocities. Thus, nTL to higher lying $n > 2$ levels is also dominant, as shown in Figs. 3-4, where TL cross sections to uncoupled $1s2snl$ states of O^{5+} are computed as a function of n (summed over all possible l-values) for a few collision energies. Such nTL-formed quartet states may now photon-decay in a cascade that will effectively feed the production of the $1s2s2p\,^4P$ state [28], thus enhancing its production. Furthermore, the $1s2s2p\,^4P_J$ state, due to its very long lifetime (0.91 ns for $J = 1/2$, 3.34 ns for $J = 3/2$ and 27.67 ns for $J = 5/2$ [27]), would be an excellent collector of such cascade products involving much faster photon decays. In particular, due to spin conservation, only $1s2snl\,^4L$ states can decay to the $1s2s2p\,^4P$ state, further simplifying the cascade sequence [29]. Such cascade schemes are well known in the literature [28]. In particular, such a cascade scenario has already been explored to some extent (only for $n = 3$) and found to be important in studies of single electron capture in low energy collisions of $O^{6+}(1s2s\,^3S)$ with He [29]. However, since all the various branching ratios for the photon transitions are not yet known, we have assumed that nTL to all the $1s2snl\,^4L$ states end up feeding the $1s2s2p\,^4P$ state with an almost 100% efficiency. This cascade TL contribution (CTL), should clearly be considered only as an *upper limit* to such cascade feeding. It is shown in Figs. 1 and 2.

As seen from Figs. 1-2, our computed CTL upper limit increases the production of $1s2s2p\,^4P$ states by a further factor of 2.5 for He and 4 for H_2, clearly establishing cascade feeding as possibly the most important contributor to the production of $1s2s2p\,^4P$ states by TL for these low-Z collision systems. Detailed calculations of transition rates and branching ratios need to be worked out for $n = 3-4$ and possibly higher n values to evaluate more precisely the cascade feeding contributions. Even the addition of the cascade feeding mechanism might not be enough to explain the remaining difference of close to a factor of 1.5 for He and 2 for H_2. Whether yet another mechanism is required to close the remaining gap between theory and experiment will remain an interesting possibility.

SUMMARY AND CONCLUSION

We have shown that the production of $O^{5+}(1s2s2p\,^4P)$ states due to TL should also consider the contributions of optical cascade (CTL) feeding from higher lying prompt states that may be produced by TL to $(1s2snl\,^4L)$ states for $n > 2$, since transfer to $n = 3-7$ is also very strong. Our rather rough CTL calculations place only an upper limit on the contributions of such a cascade feeding process resulting in much better agreement with existing

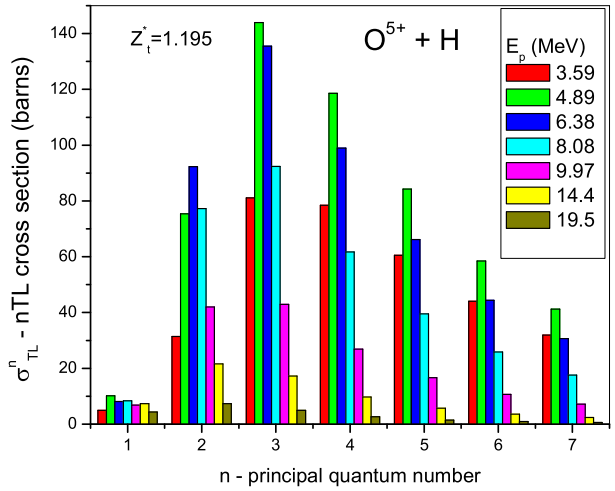

FIG. 3: (Color online). CDW calculations of nTL cross sections for the formation of uncoupled $1s2snl$ determinant states in collisions of O^{5+}+H. Bars with the same n-value correspond to different collision energies as given by the color code. An effective charge of $Z_t^* = 1.195$ was used for H to better account for the H_2 electron momentum distribution.

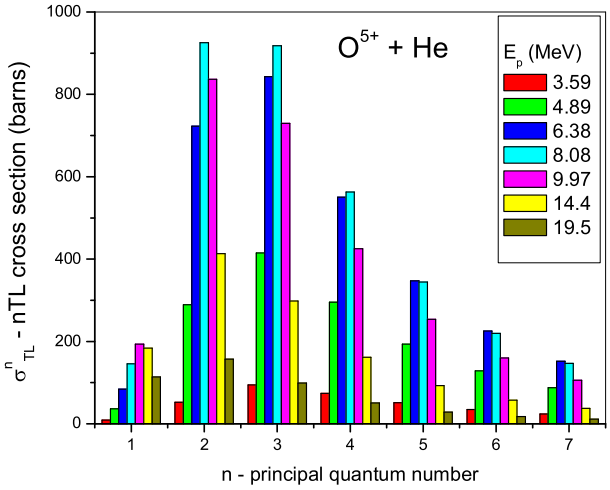

FIG. 4: (Color online). Same as for Fig. 3, but for a He target.

measurements. Clearly, a more detailed theoretical investigation of the possible cascade feeding of the $1s2s2p\,^4P$ states is needed before a more definitive quantitative understanding can be established.

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