Uncorrelated transfer excitation collisions at high energies

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A new mode of transfer excitation (TE) process in high-energy ion-atom collisions is analyzed in which two or more electrons in the target system are involved incoherently in the excitation of the projectile ion and electron transfer. This uncorrelated TE mode (UTE) is shown to resolve the long-standing discrepancy in the high-energy tail of the resonant TE (RTE) cross section in the $Nb^{31+}+H_2$ collisions, and explains satisfactorily the recent experimental studies of the system $F^{6+}+H_2$ by Schulz *et al.* [Phys. Rev. Lett. **62**, 1738 (1989)] for the uncorrelated transfer excitation followed by x-ray decay plus RTEX, involving radiative decay to a singly excited state, and of the low-lying states of F^{6+} with He by Zouros *et al.* [Phys. Rev. Lett. **62**, 2261 (1989)] for the UTE involving Auger decay.

The transfer-excitation processes (TE) in ion-atom collisions in which the target electrons and their cores play important roles in exciting the projectile ion, with the transfer of one of the target electrons to the projectile, have been vigorously studied in recent months. Although both the resonant (RTE) and nonresonant (NTE) modes of TE have been extensively investigated experimentally[1] and theoretically,[2] the role of the target electrons in exciting the projectile has never been isolated previously. In RTE, one of the electrons of the target excites the projectile and at the same time is transferred to the projectile, while in NTE the target core does the exciting as the target electrons are transferred to the projectile. Recently, an anomaly in the TE cross section was observed experimentally[3] in the $F^{6+}+H_2$ system, and it was suggested that this anomaly may be a manifestation of a third process called $2e$ TE, or the uncorrelated TE (UTE). The UTE process is mediated by two of the target electrons; one target electron excites the projectile while another electron is transferred. Since these two processes of excitation and transfer are uncorrelated, the UTE cross section could be expressed as a product of the excitation probability of the projectile and electron transfer probability. The excitation contribution was isolated recently[4] in the system $F^{6+}+He$, and in $F^{8+}+H_2$ by Schulz *et al.*[5]

The UTE was originally postulated[6] to explain the persistent discrepancies found in the analysis of high-energy tail of the RTE cross section.[1,7] More recently, a simple workable theory of all three modes of TE (RTE, NTE, and UTE) has been formulated[8] and applied[9] to the $S^{13+}+He$ system, where experimental data are available.[7] In this report, we present the result of calculations using the theory for the UTE and the inner-shell excitation[2] (ISE) without electron transfer, for the systems $F^{6+}+He$, $F^{6+}+H_2$, and $Nb^{31+}+H_2$. It is shown that the contribution of the target electrons to projectile excitation is sizable, and the theoretical prediction is consistent with the physical picture described above.

Particular interest in recent years has been on the RTE because of its close relationship to the dielectronic recombination (DR) process in electron-ion collisions. This connection has now been well established.[1,8,10–13] While DR is of importance in the study of astrophysical and laboratory plasmas, direct measurement of its cross sections was proven difficult, especially when intershell excitations are involved in the initial stage of the DR process. The RTE-DR connection has been exploited explicitly in the study of DR with intershell excitations, and at present, most of the RTE data are satisfactorily analyzed in terms of the DR cross sections and impulse approximation, where the RTE cross sections are obtained by folding the corresponding DR cross sections over the target Compton profile. Thus the TE process is schematically described as

$$\begin{aligned} &A^{Z+}+B\rightarrow[(A^{(Z-1)+})\equiv A']^{**}+B^{+} \quad \text{for TE}, \\ &A'\rightarrow(A^{(Z-1)+})+\gamma \quad \text{for TEX}, \\ &A'\rightarrow(A^{Z+})+e' \quad \text{for TEA}, \end{aligned} \tag{1}$$

where the intermediate states $(A^{(Z-1)+})$ formed by the collision decay by emission of one or more stabilizing radiations to a singly excited state (TEX) or by Auger electron emission (TEA). The TEA decay mode is generally more dominant than TEX for light projectiles, and this is reflected in large Auger yields and small fluorescence yields. Schematically we have

$$\begin{aligned} &(a+e_1)+(b+e_2+e_3)\rightarrow(a+e_1+e_2)+(b+e_3) \quad \text{for TE} \\ &\qquad\qquad\rightarrow(a+e_1)^{*}+(b+e_2+e_3) \quad \text{for ISE}, \end{aligned} \tag{2}$$

where a and b are the ion cores in A and B, and e_1, e_2, and e_3 are the electrons.

We summarize the cross section formulas for the inner-shell excitation followed by Auger decay (ISEA) and the uncorrelated transfer excitation followed by x-ray decay (UTEX) used in the following analysis. They were derived in Ref. 8.

The cross section for ISEA is defined in the impulse approximation for the target electrons in B and in the projectile rest frame; from (2), e_3 in B is regarded as a contin-

uum electron with the angular momentum l_c and thus[8]

$$\sigma^{\mathrm{ISEA}}=\sum_{d'}\frac{4\pi}{k_c^2}\int\frac{g_{d'}g_{c'}}{2g_i}A_e(d',l_{c'}\rightarrow i,l_c;p)\times W_B(|p_c-p|)dp\,\xi(d')\tau_0(\pi a_0^2)\ , \tag{3}$$

where $g_{d'}$, $g_{c'}$, and g_i are the statistical weights of the excited state d', the final state continuum c', and the initial state i, respectively. $\tau_0=2.42\times10^{-17}$ sec. In (3), W_B is the Compton profile of B, and $\xi(d')$ is the Auger yield of the state d' of A' and is related to the fluorescence yield $\omega(d')$ by $\omega+\xi=1$. A_e is the electron collisional excitation probability of the projectile A. We note[8] that A_e can be defined as analytic continuation of the Auger transition probability A_a in which one of the bound-state electrons in A_a is placed in the continuum. Thus the excitation probability A_e is obtained by analytic continuation of A_a as

$$A_e=\frac{n^3}{Z^2}A_a\bigg|_{e_n\rightarrow e_c}\ ,$$

where the continuum orbitals in A_e of (3) are energy normalized

$$R_{l_c}=\left[\frac{1}{\pi k_c}\right]^{1/2}\sin\left[k_cr+\frac{Z}{k_c}\ln 2k_cr+\cdots\right]\Big/r\ ,$$

and similarly for $R_{l_{c'}}$.

The UTEX is a new process[6,8] in which two electrons in the target B participate independently in exciting the projectile and charge transfer. That is, from (2), the excitation of A is mediated by the interaction V_{13} between electrons 1 and 3 while e_2 is transferred. (Note that the role of b in NTE is now assumed by e_3 in UTE.) The cross section is given by

$$\sigma^{\mathrm{UTEX}}=\sum_{d'}\frac{4\pi}{k_c^2}\int\frac{g''}{2g_i}A_e(d',l_{c'}\rightarrow i,l_c;p)\times W_B(|p_c-p|)dp\,\omega(d')\times|C_e|^2\tau_0(\pi a_0^2)\ , \tag{4}$$

where g'' is a combined statistical weight for the excited states of A and the scattered e_c'. $|C_e|^2$ is the electron transfer probability from B to A', defined by[8]

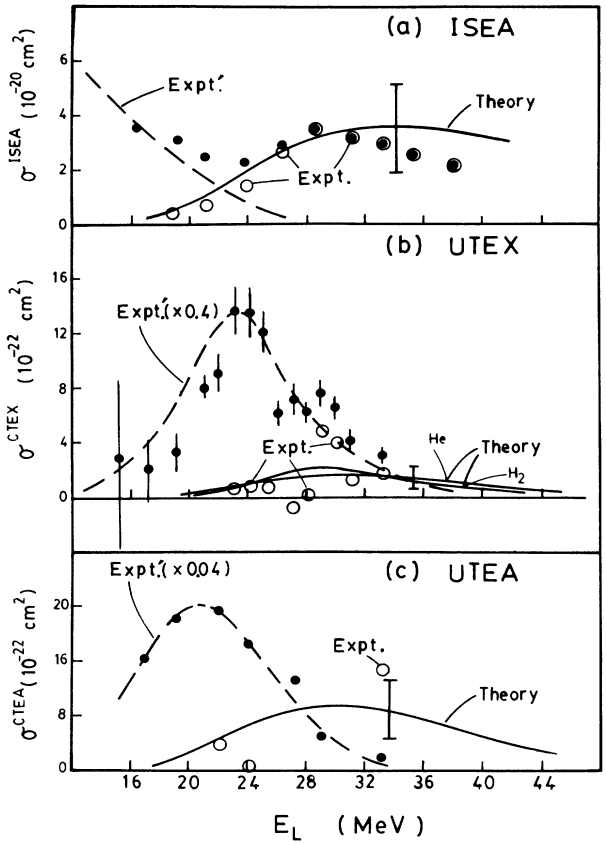

FIG. 1. (a) Cross section for the electronic projectile excitation, followed by Auger decay (ISEA) for the intermediate state $1s2s2p$ formed in the collision system $F^{6+}+He$, is compared with experimental data of Ref. 4. The dashed curve is the background contribution as estimated from experimental points; presumably, it is the contribution by the target core, as in NTE. (b) Uncorrelated transfer excitation followed by x-ray emission (UTEX) cross section for the system $F^{6+}+H_2$ is compared with the experimental data of Ref. 3. The Expt.' is actually the theoretical RTEX cross section, given in Ref. 13, reduced by a factor of 2 in order to be compared with experiment. The experimental points (○) for UTEX are obtained by subtracting the theoretical values from this adjusted experimental cross section. (c) Cross section for uncorrelated transfer excitation (theory), followed by Auger decay (UTEA) for the system $F^{6+}+He$, is compared with experimental data (○), which were obtained by subtracting the background contribution (RTEA Expt., − − −) from the total cross section (●) of Ref. 14. Estimated accuracy of the theoretical result is indicated roughly at ±50%. The total and background cross sections are reduced by 0.04 to magnify the UTEA points (○) in the figure.

$$|C_e|^2=g'\left[\frac{4}{k_c}\right]\sum_{l_c}\hat{l}_c\sum_{\lambda}\hat{\lambda}\begin{Bmatrix}l & \lambda & l_c\\ 0 & 0 & 0\end{Bmatrix}^2\left\langle R_{nl}\left|j_\lambda(pr)\frac{Z}{r}\right|R_{l_c}\right\rangle^2\left[\frac{2}{e_n-e_c}\right]^2\ , \tag{5}$$

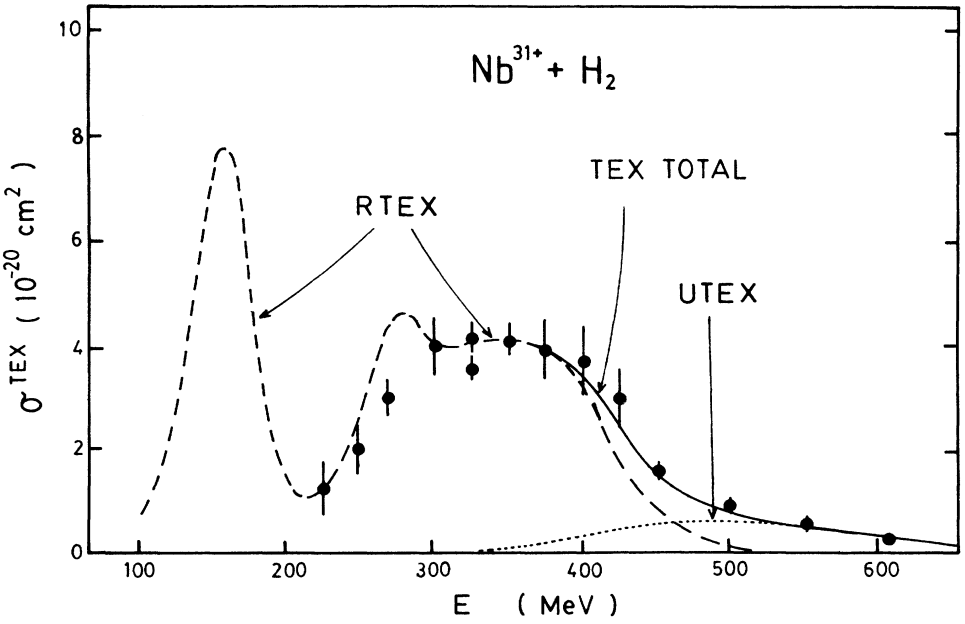

FIG. 2. The UTEX cross section is shown for the system $Nb^{31+}+H_2$, together with the RTEX (Ref. 16) and experimental cross sections from Ref. 7. The dashed curve is the theoretical RTEX cross section for Mo^{32+}, adjusted in energy for Nb^{31+}; approximately 6% downshift in E was required in accordance with the Z scaling, but hardly any changes were necessary in the magnitude and shape of the cross section obtained by folding over the Compton profile. The dotted curve is the UTEX contribution and the solid curve is the total cross section, which includes both the RTEX and UTEX contributions.

where $g'=g\hat{l}$, $\hat{l}\equiv 2l+1$, and $g=\frac{1}{2}$ or 1, depending on the intermediate states $d=1s2s^22p$ and $d=1s2s2p^2$, respectively. The formula (5) was obtained[8] by the second-order perturbation theory in closure approximation. The energies e_n and e_c are given in rydbergs.

The cross section for uncorrelated transfer excitation followed by Auger decay (UTEA) is given by a formula similar to (4), except for $\omega(d')$ replaced now by $\xi(d')$. Both factors A_e and $|C_e|^2$ are the same as those in (4) and (5).

We now discuss three recent experiments,[3,4,14] UTEX for the system $F^{6+}+H_2$ and UTEA and ISEA for the system $F^{6+}+He$. The present calculation is perhaps reliable to within a factor of 2, especially because all the electronic transition and fluorescence yields for each intermediate state d were evaluated in the simple angular momentum average scheme. Finally, we will present a definitive calculation[15] of UTEX for the $Nb^{31+}+H_2$ system.[7,16]

(i) The calculated ISEA cross section for $1s^22s \rightarrow (1s2s2p)$ is shown in Fig. 1(a) without any adjustable parameters. Contributions of different l_c states are explicitly calculated for $l_c \lesssim 6$. The experimental points (represented by the symbol ○) for ISEA are obtained from the total cross section (represented by the symbol ●) of Zouros *et al.*[4] by roughly subtracting the background (— — —). No calculation is available for this background, but presumably it is the contribution of the target core. The excitation probability A_e is calculated by modifying our MATRIX code, which was originally written for the evaluation of Auger transition probabilities. Both the incoming and outgoing electrons are completely distorted by the corresponding Hartree-Fock potentials of the ion A, with proper exchange terms included. Considering the fact that impulse approximation, isolated resonance approximation, and single configuration orbitals are used, the agreement with experimental data is reasonable. Of course, ISE is the first step in analyzing the UTE. In Fig. 1(a), the magnitude of the cross section at $E_L \lesssim 32$ MeV is consistent with experiment, but the theoretical high-energy tail is too high.

(ii) Noting the similarity between the ISE followed by x-ray decay (ISEX) and UTEX cross sections, the same A_e evaluated for ISE was used for UTE. It was found that the high-lying intermediate states ($2 \lesssim n \lesssim 6$) contribute significantly to UTE, as in previous calculations of NTE.[9] Many other intermediate states were studied to ascertain this result. For example, at $E_L=30$ MeV, the contributions from different intermediate states to the UTEX cross section are 2.15×10^{-23} cm^2 from $1s2s2p^2$, 4.58×10^{-23} cm^2 from $1s2s2p3p$, and 3.39×10^{-23} cm^2 from $1s2s2p4p$. The capture probability $|C_e|^2$ used here is the same as that evaluated for NTE earlier.[9] The result is compared with experimental data[3] in Fig. 1(b). The UTEX cross section (○) is obtained by subtracting the background cross section[13] (— — —) from the experimental data of Ref. 3. The experimental points are scattered and it is difficult to assess the effect of UTEX more accurately.

(iii) Calculation of the cross section for UTEA is similar to that for the UTEX, with the fluorescence yield ω replaced by the Auger yield ξ. The theoretical cross section for UTEA is well within the uncertainty of the ex-

perimental points[14] as deduced by subtracting the resonant mode of TEA (RTEA) contribution from the overall experimental data [Fig. 1(c)].

(iv) Finally, the UTEX for the system $Nb^{31+}+H_2$, in which the $2p$ excitation is dominant, is studied[15] (Fig. 2). The earlier calculation[16] of the resonant mode of TEX (RTEX) is shown, together with the accurate experimental data of Tanis *et al.*[7] and the UTEX contribution. This case thus provides the decisive confirmation of the UTEX.

A preliminary result of our calculations of the ISEA, UTEX, and UTEA processes is presented. Considering the complexity of the calculations involved and the approximations used, the agreement with experimental data is satisfactory. The assignment of the UTEX data by Schulz *et al.* as $2e$ TE ($\equiv$UTE) is consistent with our calculation, and the ISEA and UTEA data by Zouros *et al.* are explainable in terms of our result. The experiment at high energy of Zouros *et al.*[14] as shown in Fig. 1(c), is explained by the UTEA, but the data are not accurate enough to make a detailed comparison. On the other hand, the related experiment of Schulz *et al.*[5] for the $F^{8+}+H_2$ system gives a clear indication of the UTEA. The comparison in the case of $Nb^{31+}+H_2$ is definitive. The general structure of the theory seems to be correct, reflecting properly all the physics of the various modes.

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