PHYSICAL REVIEW A VOLUME 10, NUMBER 3 SEPTEMBER 1974

K-vacancy production in symmetric heavy-ion collisions*

W. E. Meyerhof†
Department of Physics, Stanford University, Stanford, California 94305
(Received 19 February 1974; revised manuscript received 13 May 1974)

Recent calculations of Thorson and co-workers for $H^+ + H$ ionization mechanisms and the Briggs-Macek scaling law for K-vacancy production in symmetric heavy-ion collisions are used to show the following: (1) If Fano-Lichten–type electron promotion is inhibited because of the absence of a $2p$ vacancy, i.e., if $Z > 10$, K vacancies in symmetric collisions are produced mainly by $2p\sigma$ electron excitation to vacant bound and unbound molecular-orbital states. (2) The direct $1s\sigma$ excitation cross section to vacant bound and unbound states can be obtained experimentally. The relationship between atomic and molecular-orbital Coulomb excitation cross sections is discussed.

K-vacancy formation in heavy-ion collisions is not only of intrinsic interest,[1,2] but also is important in the generation of molecular-orbital (MO) K x rays[3] and positrons[4] in energetic heavy-ion collisions. For light ions ($Z \leqslant 10$) it is well established[1,2] that Fano-Lichten–type electron promotion[5] provides the basic mechanism of $1s$ vacancy production: If a $2p\pi$ vacancy is available early in the collision (inset, Fig. 1) an electron can be promoted from the $2p\sigma$ to the $2p\pi$ MO, leaving a vacancy in the $2p\sigma$ MO. This vacancy is shared between the separating collision partners.[6] The present paper attempts to demonstrate two main points. (i) If the Pauli exclusion principle inhibits the presence of a $2p\pi$ vacancy early in the collision, i.e., for $Z > 10$,[7] the most probable process of K-vacancy formation is by $2p\sigma$ electron excitation to high-lying vacant and to continuum MO states. (ii) It is possible to determine experimentally the cross section for direct $1s\sigma$ electron excitation to vacant states.

The arguments rely on a recent MO calculation of ionization cross sections in $H^+ + H$ collisions[8] and on a scaling law for K-vacancy-production cross sections in symmetric heavy-ion collisions.[9,10] Figure 1 shows cross sections computed for three $1s$ excitation processes in slow $H^+ + H$ collisions, using MO wave functions: (a) from the $1s$ to the $2p$ state via $2p\sigma$-$2p\pi$ coupling[5] in the $(H_2)^+$ system,[9,11-13] (b) from the $1s$ state to the continuum via the *ungerade* MO ($2p\sigma$, dynamically mixed with $2p\pi$),[8] and (c) from the $1s$ state to the continuum via the *gerade* MO ($1s\sigma$).[8] As shown in Fig. 1, at low projectile energies these cross sections differ from each other by many orders of magnitude, hence should be experimentally quite distinct. Figure 1 gives some experimental $H^+ + H$ excitation[14] and ionization[15] and $H^+ + H_2$ ionization[16,17] cross sections.

Briggs and Macek[9] have derived a scaling law for the K-vacancy-production cross section σ_K in a symmetric collision by process (a), which is equally valid for other $1s$ excitation processes if shielding effects due to the outer electrons are ignored,[10] and which can be written

$$Z^2\sigma_K(E_1) = F_B(E_1/M_1Z^2) \approx F(E_1/\lambda U) \ , \tag{1}$$

where E_1 and M_1 are projectile (lab) energy and mass, $\lambda = M_1/m$ (m = electron mass), and U is the K binding energy. For accurate scaling the value of Z should be adjusted slightly,[9] but for the present purpose of order-of-magnitude comparisons this is not necessary. Also[9] the functional form of F_B should be compared to the $^2H^+ + ^2H$ system, rather than to $H^+ + H$ as is done below, but this is important only very close to the excitation threshold. The second functional form of F in Eq. (1), which is used below, is familiar from binary-encounter theory[1] and resembles closely Born-approximation scaling[18] for symmetric collisions.

Figure 2 compares experimental K-vacancy-production cross sections scaled according to Eq. (1) with the curves transposed from Fig. 1. The curves are multiplied by 4 because there are four $1s$ electrons in a heavy-ion collision, compared to one in $H^+ + H$. For $Z \leqslant 10$ only Auger electron measurements are presented[19,20]; the experimental cross sections have been multiplied by a factor $f = 12/N_v$, where N_v is the total number of $2p$ vacancies in the collision partners, because curves (a) assume two $2p\pi$ vacancies whereas in the collision of two atoms with $Z \leqslant 10$ the vacancy availability is[9] equal to $\frac{1}{6}N_v$. As previously shown in Ref. 9 the data for $Z \leqslant 10$ scale reasonably well to curves (a), demonstrating that the Fano-Lichten process[5] operates here.

For $Z > 10$ only gas-target data[21-23] are given in Fig. 2 in order to avoid complications from multiple collision processes in solid targets.[7] Since for vacant states the vacancy availability is identical for $H^+ + H$ and for symmetric heavy ions, f is set equal to unity. The $Cl^+ + Ar$ data

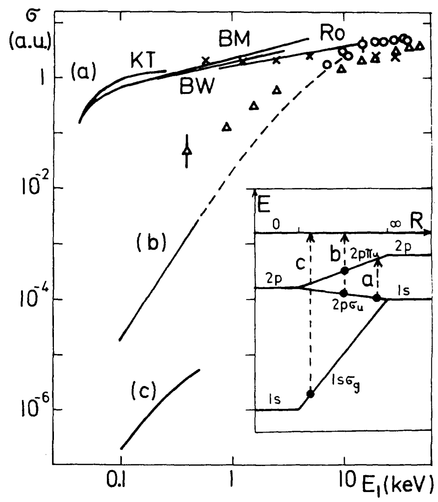

FIG. 1. Cross sections for 1*s* electron excitation in $H^+ + H$ collisions as a function of proton (lab) energy (1 a.u.$=2.8\times10^{-17}$ cm^2). (a) 1*s*-2*p* excitation via $2p\sigma$-$2p\pi$ coupling. Theoretical curves: BW—Ref. 12, KT—Ref. 11, Ro—Ref. 13, BM—Ref. 9 (this cross section, calculated effectively for two 1*s* electrons, has been reduced by one-half). Experimental data: *X*—Ref. 14. (b) 1*s*-continuum excitation via *ungerade* MO. Theoretical curve: Ref. 8; this has been extrapolated arbitrarily to meet the data of Ref. 15. Experimental data: O—Ref. 15; Δ—one-half of $H^+ + H_2$ ionization cross section from Refs. 16 and 17. (c) 1*s*-continuum excitation via *gerade* MO. Theoretical curve: Ref. 8. Inset gives schematic MO levels and indicates symbolically the transitions between them corresponding to curves (a), (b), and (c).

of Ref. 21 are treated as "symmetric" because in the energy range investigated the Cl/Ar *K* x-ray ratio was not far from unity. The Cl *K* x-ray cross sections have been corrected for the neutral fluorescence yield[24] and doubled. At low bombarding energies the scaled experimental data is *several orders of magnitude* below curve (a) and follows the trend of curve (b), suggesting that some $2p\sigma$ electron excitation to the continuum takes place. There could be several reasons why most of the data lie above curve (b), which have to be evaluated by further work. (1) In addition to $2p\sigma$ excitation to the continuum, there can be excitations to bound vacant states.[22] There is presently no reliable way to estimate these. (2) There could be multistage excitation processes, such as radial coupling of vacant projectile states to the $2p\pi$ MO early in the collision, providing a $2p\pi$ vacancy which can be filled by promotion of a $2p\sigma$ electron. Crude estimates for such a process[25] indicate possible large contributions to the observed cross section. (3) The scaling law as applied here may not be very accurate.[9] (4) The $H^+ + H$ calculations[8] may not be accurate.

An experimental estimate of the $1s\sigma$ cross section [curve (c) in Fig. 1] can be obtained from the following considerations. In Fig. 3(a) the MO levels relevant to an asymmetric collision are shown. A vacancy made in the $1s\sigma$ MO appears as a 1*s* vacancy of the higher-*Z* collision partner. In addition, if the collision is not too asymmetric, the $1s(H)$ state can obtain a vacancy from the $2p\sigma$ MO, as discussed in Ref. 6 where the probability *w* of vacancy transfer from the $2p\sigma$ to the $1s\sigma$ MO is evaluated. Figure 3(b) gives the *K*-vacancy thick-target yield $y(H)$ of the higher-*Z* collision partner for collisions with 47-MeV I projectiles[26] as a function of the charge asymmetry $Z_H - Z_L$ between the higher- and lower-*Z* collision partners. Close to symmetry, feeding from the $2p\sigma$ state dominates the higher-*Z* vacancy yield, as shown by the solid calculated curve. Far from symmetry, the yield deviates from this curve because direct $1s\sigma$ excitation becomes dominant.[27] Extrapolation to $Z_H - Z_L = 0$ (dashed line) should give a rough estimate for the $1s\sigma$ excitation yield for a symmetric collision. This procedure was followed, after first converting yields to cross sections, in ob-

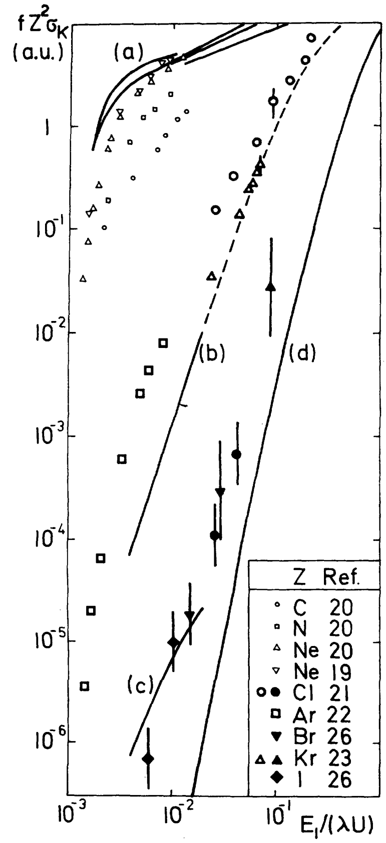

FIG. 2. Scaled *K*-vacancy-production cross sections versus reduced projectile energy. Curves (a), (b), and (c) from Fig. 1, but multiplied by 4 (see text). Curve (d) from Ref. 29, with $Z_1 = Z_2 = 1$. See text for definition of factor *f*.

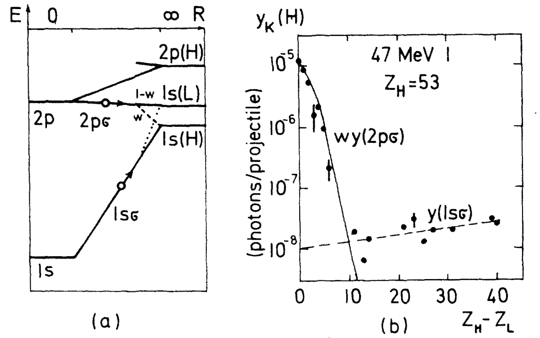

FIG. 3. (a) Schematic MO levels for an asymmetric collision. See Ref. 6 for evaluation of $2p\sigma$-$1s(H)$ vacancy transfer probability w. (b) Projectile thick-target K-vacancy yield for 47-MeV I beam. The solid curve gives the expected vacancy feeding of the $1s(H)$ state from the $2p\sigma$ level; $y(2p\sigma)$ is the total $2p\sigma$ vacancy yield (Ref. 6), $y(1s\sigma)$ is the yield assigned to direct $1s\sigma$ excitation.

taining the points shown with solid symbols in Fig. 2. Despite the rough extrapolation procedure, the points lie near the scaled curve for process (c), suggesting that indeed they represent $1s\sigma$ excitation to the continuum, and perhaps to vacant bound states. Using now curve (c) in order to estimate an upper limit for the expected $1s\sigma$ vacancy production cross section in U + U collisions,[4] one finds $\sigma_K \simeq 30$ and 800 mb at $E_1 = 600$ and 1600 MeV (lab), respectively. The positron-emission[4] cross section is then estimated to be 0.0016 and 1.3 μb at these energies,[28] considerably lower than in Ref. 4.

Relation to atomic Coulomb excitation. Atomic Coulomb excitation calculations[18] can be corrected approximately for projectile scattering and target binding-energy change,[29] but always produce dominant $1s$ to continuum s state transitions at low projectile velocities.[30] Hence this treatment misses the important role[8] of the $1s$ to continuum p state transitions caused by rotational coupling in MO calculations. At high projectile velocities, the MO treatment gives the same result as the Born approximation.[31] These statements are borne out qualitatively by curve (d) in Fig. 2, obtained by setting $Z_1 = Z_2 = 1$ in the expressions of Ref. 29. Quantitative agreement cannot be expected since these expressions have been computed only for $Z_1 \ll Z_2$.

This work was stimulated by a private communication from W. Thorson. Discussions with R. Anholt, W. Brandt, C. Melius, E. Merzbacher, and T. Saylor, and results prior to publication from F. Saris and B. Fastrup are gratefully acknowledged.

*Supported in part by the National Science Foundation.
†On part-time leave at Nuclear Chemistry Division, Lawrence Berkeley Laboratory, Berkeley, Calif. 94704.

[1]J. D. Garcia, R. J. Fortner, and T. M. Kavanagh, Rev. Mod. Phys. 45, 111 (1973).

[2]Q. C. Kessel and B. Fastrup, Case Studies in Atomic Physics 3, 137 (1973).

[3]W. E. Meyerhof *et al.*, Phys. Rev. Lett. 30, 1279 (1973); 32, 502 (1974); 32, 1279 (1974).

[4]K. Smith *et al.*, Phys. Rev. Lett. 32, 554 (1974); cross sections in this paper should be multiplied by 10^{-4} [J. Rafelski (private communication)].

[5]W. Lichten, Phys. Rev. 164, 131 (1967).

[6]W. E. Meyerhof, Phys. Rev. Lett. 31, 1341 (1973).

[7]With a solid target, multiple collisions can produce $2p\pi$ vacancies, followed by $2p\sigma$-$2p\pi$ promotion, even for $Z > 10$. See F. W. Saris and D. J. Bierman, Phys. Lett. A 35, 199 (1971); R. C. Der *et al.*, Phys. Rev. Lett. 27, 1631 (1971); M. O. Lutz *et al.*, Phys. Rev. Lett. 28, 8 (1972); T. K. Saylor (private communication).

[8]V. SethuRaman, W. R. Thorson, and C. F. Lebeda, Phys. Rev. A 8, 1316 (1973).

[9]J. S. Briggs and J. Macek, J. Phys. B 5, 579 (1972); 6, 982 (1973) [in Eqs. (18) and (21) Z^2 should be replaced by Z^{-2}].

[10]W. R. Thorson (private communication).

[11]S. K. Knudson and W. R. Thorson, Can. J. Phys. 48, 313 (1970).

[12]D. R. Bates and D. A. Williams, Proc. Phys. Soc. Lond. 83, 425 (1964).

[13]H. Rosenthal, Phys. Rev. Lett. 27, 835 (1971).

[14]E. W. Thomas, *Excitation in Heavy Particle Collisions* (Wiley-Interscience, New York, 1972), p. 99.

[15]W. L. Fite *et al.*, Phys. Rev. 119, 663 (1960).

[16]H. B. Gilbody and J. B. Hasted, Proc. R. Soc. A 240, 382 (1957).

[17]E. S. Solovev *et al.*, Zh. Eksp. Teor. Fiz. 42, 659 (1962) [Sov. Phys.—JETP 15, 459 (1962)].

[18]E. Merzbacher and H. W. Lewis, *Handbuch der Physik*, (Springer Verlag, Berlin, 1958), Vol. 34, p. 166.

[19]R. K. Cacak, Q. C. Kessel, and M. E. Rudd, Phys. Rev. A 2, 1327 (1970).

[20]E. Boving and B. Fastrup (unpublished).

[21]L. Winters *et al.*, Phys. Rev. Lett. 31, 1344 (1973).

[22]F. W. Saris *et al.*, J. Phys. B (to be published).

[23]R. Anholt *et al.* (unpublished).

[24]W. Bambynek *et al.*, Rev. Mod. Phys. 44, 716 (1972).

[25]W. E. Meyerhof, in Third International Seminar on Ion-Atom Collisions, Gif-sur-Yvette, France, 1973 (unpublished).

[26]W. E. Meyerhof *et al.*, Bull. Am. Phys. Soc. 18, 559 (1973); and to be published.

[27]In direct $1s\sigma$ excitation, multiple collisions can play no role [see Fig. 3(a)]. Also, the projectile K yield, shown in Fig. 3b, is unaffected by target recoil effects. See K. Taulbjerg, B. Fastrup, and E. Laegsgaard, Phys. Rev. A 8, 1814 (1973).

[28]W. E. Meyerhof, Bull. Am. Phys. Soc. 19, 663 (1974).

[29]G. Basbas, W. Brandt, and R. Laubert, Phys. Rev. A 7, 983 (1973).

[30]J. Bang and J. M. Hansteen, Mat. Fys. Medd. Dan. Vid. Selsk 31, No. 13, 1 (1959).

[31]D. R. Bates, in *Atomic and Molecular Processes*, edited by D. R. Bates (Academic, New York, 1972), p. 594.