from electron 2. The matrix element in Eq. (3.29) then takes the form

$$g(2p_0 \to 2p_{\pm 1}) = (R^{\rm H}_{2p}(r_1)\, Y_1^{\pm 1}(\hat{r}_1),\, \hat{k}\cdot[\tfrac{15}{2}\,\hat{R}_1(\hat{R}_1\cdot\vec{r}_1)^2 - \tfrac{3}{2}\hat{R}r_1^2 - 3\vec{r}_1(\hat{R}\cdot\vec{r}_1)]\, R^{\rm H}_{2p}(r_2)\, Y_1^0(\hat{r}_1)) \;. \qquad \text{(C3)}$$

We have

$$(Y_1^{-1}(\hat{r}_1),\, (\hat{R}_1\cdot\vec{r}_1)^2\, Y_1^0(\hat{r}_1)) = r_1^2 \int Y_1^{-1}(\hat{r}_1)^*\, [\cos\gamma\cos\theta_1 + \sin\gamma\cos\theta_1\cos\varphi_1]^2\, Y_1^0(\hat{r}_1)\, d\hat{r}_1 = (\sqrt{2}/5)\, r^2\cos\gamma\sin\gamma \;, \qquad \text{(C4)}$$

$$(Y_1^{-1}(\hat{r}_1),\, (\hat{k}\cdot\vec{r}_1)(\hat{R}_1\cdot\vec{r}_1)\, Y_1^0(\hat{r}_1)) = r_1^2 \int Y_1^{-1}(\hat{r}_1)^* \cos\theta_1[\cos\gamma\cos\theta_1 + \sin\gamma\sin\theta_1\cos\varphi_1]\, Y_1^0(\hat{r}_1)\, d\hat{r}_1 = r^2\sin\gamma/5\sqrt{2} \;. \qquad \text{(C5)}$$

This then leads to

$$g(2p_0 \to 2p_{\pm 1}) = (3/\sqrt{2})\sin\gamma\,[\cos^2\gamma - \tfrac{1}{5}] \times (R^{\rm H}_{2p}(r_1),\, r_1^2 R^{\rm H}_{2p}(r_1)) \;, \qquad \text{(C6)}$$

which is equivalent to Eq. (3.30).

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Deduction of Heavy-Ion X-Ray Production Cross Sections from Thick-Target Yields

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The conventional formula determining x-ray production cross sections from thick-target yields has to be corrected for the effects of energy-loss straggling, x rays from recoil atoms, and nonstraight ion trajectories when heavy (keV and low MeV) ions are used as projectiles. The first two corrections are evaluated in this paper for the case where the last is small (negligible absorption). Carbon K x-ray cross sections are deduced from published yield data. Large corrections, up to one order of magnitude, are found.

I. INTRODUCTION

When heavy ions slow down in gaseous or solid targets inner-shell excitations are created in violent collisions even at velocities $v < e^2/\hbar$.[1] Characteristic x-ray production cross sections σ_x of the order of up to almost 10^5 b have been reported.[2,3] As a function of ion energy E, the reported cross sections rise steeply from a rather well-defined threshold energy[2,4] U. At higher energies, σ_x increases more slowly with energy. Eventually, a dropoff of σ_x at still higher energies must be expected, similar to the case of light ions at velocities[5] $v \gg e^2/\hbar$.

Experimentally, cross sections were determined either directly, in gas targets under single-collision conditions,[2] or indirectly, on thick solid targets where the ion beam is stopped completely.[2-4] It is of particular interest to compare x-ray production cross sections from ions slowing down in gaseous and solid targets of the same element. Precise determination of the cross section from a thick-target yield is, therefore, of considerable importance. In the present communication we are concerned with this latter problem. Care has to be taken of the slowing-down characteristics of the ion beam, the absorption of x rays in the target, and the possible contribution to the x-ray yield of secondary collisions undergone by recoiling atoms. In addition, the assignment of the obtained cross section to any particular charge state of the moving ions must be taken with caution.

The evaluation of existing data[2,3,6,7] has been based on the following formula, derived for fast protons[8]:

$$\sigma_x(E) = S(E)\frac{dI(E)}{dE} + \frac{\mu}{N}\, I(E) \ , \tag{1}$$

where E is the initial ion energy, $I(E)$ the observed thick-target yield, $S(E)$ the stopping cross section of the ion, N the density of target atoms, and μ the absorption coefficient of the characteristic x rays. In order that Eq. (1) be valid, the following assumptions must be fulfilled: (i) The ions slow down along straight trajectories. (ii) There is a unique relation of energy vs depth. (iii) Recoil atoms do not produce x rays in subsequent collisions. (iv) There is a unique charge state of the ion as a function of energy, and $\sigma_x(E)$ is the cross section corresponding to that charge state. The significance of these four assumptions depends on the ion-target combination, the ion energy, and the particular transition considered.

At sufficiently low ion energy, and in particular for low mass ratio M_2/M_1 (M_1 = ion mass, M_2 = target mass), ion penetration depths are small enough[9] for the absorption term in Eq. (1) to be unimportant. Then assumption (i) reduces to the requirement that no appreciable fraction of the ions is backscattered. Backscattering coefficients have been shown[10] to be small except for $M_2/M_1 \gg 1$.

Assumption (ii) cannot be fulfilled rigorously because of energy-loss straggling. In view of the strong energy dependence of $\sigma_x(E)$, an excess energy (at any particular depth) will give a pronounced increase in the x-ray yield, which will not be compensated by the corresponding decrease due to those ions that have less than average energy (at the same depth).

Assumption (iii) is of interest only when *target* x rays are observed. Its importance is determined by first of all the relative significance of nuclear as compared to electronic stopping. We shall demonstrate that the correction to Eq. (1) due to recoil atoms may be exceedingly large. In some cases (e.g., Kr→C), Eq. (1) may overestimate σ_x by an order of magnitude or more. As a qualitative argument, we note that heavy ions slowing down in light targets can create recoil atoms with velocities up to almost twice as large as that of the ion. The energy of heavy ions is spent predominantly in creating recoil atoms, even in the upper keV region, while light atoms lose a substantial part of their energy in electronic excitation, even in the lower keV region.[11] Hence, although the cross section for inner-shell excitations need not follow quantitatively the total electronic stopping cross section (because of the threshold nature of x-ray emission), recoil x rays cannot in general be ruled out beforehand as a significant contribution.

Assumption (iv) is doubtful when the x-ray production cross section depends sensitively on the charge state since we normally deal with a *distribution* of charge states of ions slowing down in solids.[12] Then, $\sigma_x(E)$ as determined from Eq. (1) is to be understood as an average over different charge states. This average need not necessarily be taken over the equilibrium distribution of charge states. Especially near threshold, most x rays may be produced before equilibrium is established. Bombardment experiments near threshold at different ionic charges are of interest to test this latter point.

II. BASIC EQUATION

In the present communication we restrict our attention to the case $M_2/M_1 \lesssim 1$, where ion backscattering is negligible,[10] and penetration depths $R_p(E)$ are small except at very high energies,[9] i.e.,

$$\mu R_p(E) \ll 1 \ . \tag{2}$$

In the case of observed target x rays, it is noteworthy that also the loss of recoil energy through the surface is small.[13] Then, $I(E)$ is the average number of x-ray quanta (of a particular transition) created during the slowing down of an ion from energy E to zero in an infinite medium. $I(E)$ is connected to the x-ray production cross section for ion-target collisions $\sigma_x(E)$ by an integrodifferential equation typical for cumulative radiation effects[11]

$$\int d\sigma\,[I(E) - I(E-T)] + S_e(E)\frac{dI(E)}{dE} = \sigma_x(E) + \int d\sigma\, I_R(T) \ , \tag{3}$$

where $d\sigma = d\sigma(E,\ T)$ is the differential cross section for an elastic collision with the energy transfer T, $S_e(E)$ the electronic stopping cross section of the ion, and $I_R(T)$ the average production of x rays by a recoil atom of energy T. The influence of the charge state on $d\sigma$ and $S_e(E)$ is assumed to be small, and $\sigma_x(E)$, as above, is understood as an average cross section over the distribution of charge states.

Equation (3) implies, in addition to Eq. (2) being valid, that (a) slowing down is by random collisions, (b) electronic and nuclear collisions are decoupled, and (c) the lifetime of an inner-shell excited state is short as compared to the time interval between two comparable excitations.

Assumption (a) is mainly a matter of geometry. Pronounced channeling effects have been observed on single crystals when (a) was not fulfilled.[14,15]

Assumption (b) appears at odds in the present context, at least at first sight. We note, however, that the assumption is needed only to determine the *slowing-down behavior* rather than the *x-ray production cross section*. It is well known from the theory of ion ranges and energy deposition[9,11] that assumption (b) can be well justified since the contribution of close collisions to electronic stopping is relatively small.

Assumption (c) is worth while mentioning since nonlinear terms in $I(E)$ would enter in Eq. (3) if (c) were not fulfilled, just as in hot-atom chemistry.[16] X-ray and, more important, Auger lifetimes are short enough to ensure validity of assumption (c).[1]

Three special cases of Eq. (3) are of interest: (i) When only *ion* x rays are measured, we have

$$I_R(T) \equiv 0 \ . \tag{4}$$

(ii) Equation (3) stands as it is when *target* x rays are observed. (iii) In the special case of self-bombardment (e.g., $Cu^+ \to Cu$), we have

$$I_R(E) \equiv I(E) \ . \tag{5}$$

If we first assume continuous slowing-down,[9] i.e., expand the integral on the left-hand side of Eq. (3) up to the first term in T, and, secondly, neglect the recoil term on the right-hand side, we obtain

$$[S_n(E) + S_e(E)] \frac{dI(E)}{dE} = \sigma_x(E) \ , \tag{6}$$

where $S_n(E) = \int T\, d\sigma$ is the nuclear stopping cross section. Equation (6) is identical with Eq. (1) for $\mu = 0$ [see Eq. (2)].

The case of non-negligible absorption and/or backscattering is more involved, since it requires integral equations of the type discussed in Ref. 17, containing spatial coordinates.

III. EVALUATION

Although Eq. (3) could be solved for $I(E)$ when I_R, $d\sigma$, and S_e are known, the most common situation will be that $I(E)$ is known, and $\sigma_x(E)$ is to be determined, $d\sigma$ and S_e being given more or less accurately. $\sigma_x(E)$ can then be evaluated by numerical integration. Analytical approximation formulas are desirable, though. We note that if *target* x rays are measured, the recoil term $I_R(E)$ must be known, preferably from experiment.

In many cases the experimental $I(E)$ curves can be fitted to the expression

$$I(E) = I_0(E/U^* - 1)^P \ , \tag{7}$$

with $P \sim 2$ (Table I). The same interpolation formula can be used for $I_R(E)$, with parameters I_{R0}, U_R^*, and P_R.

The recoil term on the right-hand side of Eq. (3) is normally made up of contributions from a rather limited T interval. It is then sufficiently accurate in the evaluation to use the cross section[18]

$$d\sigma = CE^{-m} T^{-1-m}\, dT \ , \quad 0 < m < 1 \ . \tag{8}$$

The integral then reads

$$\int d\sigma I_R(T) = I_{R0}\, C(EU_R^*)^{-m} B_{1-U_R^*/T_m}(P_R + 1,\ m - P_R) \ , \tag{9}$$

where $B_p(x,\ y)$ is the incomplete beta function[19] and T_m is the maximum energy transfer. m and C should be chosen in accordance with the ion energy.[17,18]

The discussion of the integral on the left-hand side of Eq. (3) will be done in two parts.

A. Initial Energy Well above Threshold

Provided that E is large compared to the threshold U^* of the $I(E)$ function, we can neglect threshold effects in the integrations on the left-hand side of Eq. (3). Expanding in powers of T, the left-hand side reads

$$[S_n(E) + S_e(E)] \frac{dI(E)}{dE} + \tfrac{1}{2} W(E) \frac{d^2 I(E)}{dE^2} + \cdots \ , \tag{10}$$

where

$$W(E) = \int T^2 d\sigma \ . \tag{11}$$

Higher terms include the subsequent moments of $d\sigma$. From Eq. (7) one concludes that for $E \gg U^*$, and $P \approx 2$, the third derivative of $I(E)$ will be small, and the truncated expansion (10) sufficiently accurate. In the case of very different masses, the series (10) converges rapidly, just because

$$T \lesssim T_m = \gamma E \ll E \ , \tag{12}$$

$$\gamma = \frac{4M_1 M_2}{(M_1 + M_2)^2} \ . \tag{12a}$$

Tabulations of $S_n(E)$ and $W(E)$ for the Thomas-Fermi interaction can be found in Ref. 18, together with simple formulas which are useful when another screened Coulomb interaction should be adopted. For $S_e(E)$, one can use analytical predictions[9,11] or, preferably, experimental values.[20]

B. Initial Energy near Threshold

In the energy interval

$$U^* \lesssim E \lesssim U^*/(1 - \gamma) \tag{13}$$

TABLE I. Parameters P, U^*, and I_0 giving best fit of Eq. (7) to experimental $I(E)$ curves.

Incident ion	U^* (keV)	P	$10^5 I_0$	E_{max}(keV)
C	12	1.756	7.134	200
N	13	1.988	3.081	100
O	14	2.410	1.000	100
Ne	15	2.469	0.2250	120
Ar	18	2.262	3.003	200
Kr	25	2.429	0.3458	>80
Xe	20	3.463	0.01916	>80

the expansion (10) is not rigorous as it stands although it is expected to be reasonably accurate except for E very close to U^*. The good accuracy is due to the fact that mostly *small* values of T contribute to the integral. It can be evaluated exactly if Eqs. (7) and (8) are valid. We then obtain

$$\int d\sigma[I(E) - I(E-T)] = (1/m)CE^{-2m}I(E) \times [PB(1-m, P)(1-U^*/E)^{-m} - \gamma^{-m}], \quad (14)$$

where $B(x, y)$ is the complete beta function.[19] Equation (14) is useful when the threshold value U of $\sigma_x(E)$ has to be found.

IV. EXAMPLES

As an illustration, we have calculated the cross sections for carbon K x-ray production in collisions

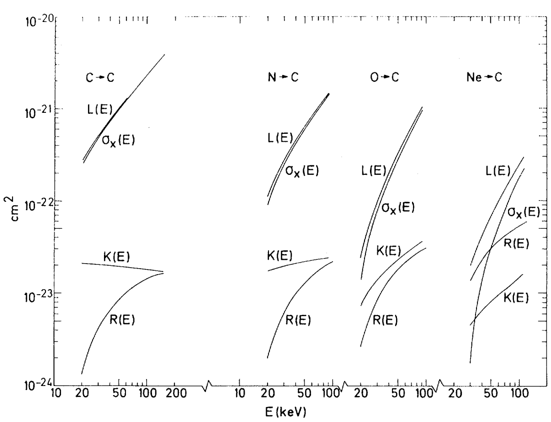

FIG. 1. Carbon K x-ray production cross section as a function of the energy of the incident ion. Absorption is neglected. $\sigma_x(E)$ follows from Eq. (3) up to the second term in the expansion (10). $L(E)$ is the cross section according to Eq. (1). We have repeated the evaluation of the $L(E)$ term analogous to Ref. 3, obtaining slightly different results. $K(E) = \frac{1}{2}W(E)(d^2I/dE^2)$ and $R(E) = \int d\sigma\, I_R(T)$. $R(E)$ is based on power cross sections with values of m and λ_m [λ_m determines C (Ref. 17)] to obtain best fit to Thomas-Fermi differential cross section in the energy range of interest. For all ion-target combinations on this graph, we used $m = 0.917$ and $\lambda_m = 0.327$.

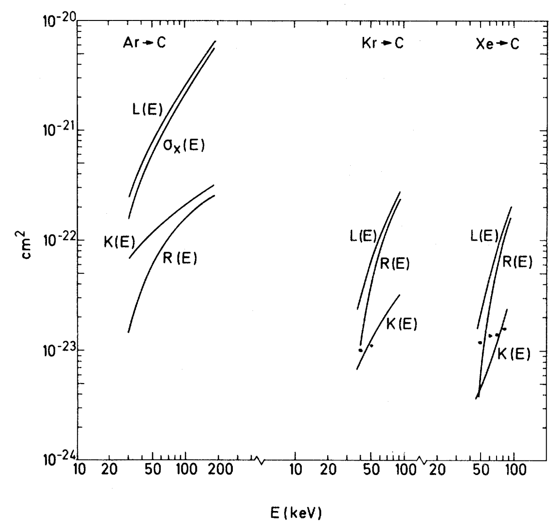

FIG. 2. Same as Fig. 1. (m; λ_m) = (0.8; 0.248) for Ar, (0.576; 0.335) for Kr, and (0.5; 0.430) for Xe. In the cases of Kr and Xe, we have not drawn a curve of $\sigma_x(E)$ but just indicated by circles that the error in the small quantity $\sigma_x(E)$ is so much enhanced that a correct determination of $\sigma_x(E)$ is impossible.

involving various ions incident on amorphous carbon. In the low-energy region, where absorption can be neglected, the existing data[3,6] fit very well to Eq. (7). The parameters giving the best fit are listed in Table I, together with the energy E_{max}, below which the fit is good to within 5%. This accuracy is consistently within the experimental accuracy given in Refs. 3 and 6.

In the evaluation we used the Thomas-Fermi values for $S_n(E)$ and $W(E)$, as given in Ref. 18, and in the recoil term, the power cross section (8) with the constants m and C giving the best fit to the Thomas-Fermi differential cross section in the range of energies of interest. The results are given in Figs. 1 and 2. It is seen that the corrections to Eq. (1) are rather small for C, N, and O ions, except for low-energy oxygen, where the straggling correction becomes as much as 30%. In the case of neon, we have a large recoil correction, especially at the lowest energies, whereas for argon, a noticeable correction only occurs at low energies from the straggling term. For both krypton and xenon, the recoil correction becomes so large that an accurate determination of $\sigma_x(E)$ does not appear feasible within the accuracy of our analysis and the existing input parameters. Note especially that the resulting cross section for Kr shows a decrease with increasing energy, which is almost certainly an artifact of the evaluation. The analysis of the Kr and Xe data obviously does not give more than an order of magnitude estimate of $\sigma_x(E)$.

It is fairly obvious that the threshold value of the thick-target yield is determined by recoil x rays in the case of neon, while in the cases of nitrogen, oxygen, and argon, the threshold behavior seems to be governed by $\sigma_x(E)$.

V. DISCUSSION

It is of interest to have simple qualitative criteria concerning the relative importance of the two corrections discussed in this paper.

The energy-straggling correction is most significant when the mass ratio M_2/M_1 is not too different from 1. But small values of the direct excitation cross section $\sigma_x(E)$ result in a relatively high recoil contribution; the energy-straggling correction may therefore be important even if it is small at first sight. When the recoil term is small, both corrections are unimportant in the case of dominant electronic stopping.

As to the magnitude of the two corrections, we have not found any situation where the straggling correction was prohibitively large; yet, the recoil contribution may dominate the thick-target yield to such a degree that only an upper limit to $\sigma_x(E)$ can be determined from the data. We have shown that this upper limit may be smaller by an order of magnitude than the $\sigma_x(E)$ values found in previous evaluations.[6]

From the above considerations it follows that Eq. (1) can be used to evaluate $\sigma_x(E)$ from thick-target yield data when the electronic stopping dominates over the nuclear stopping. When looking for target x rays, one must also demand that the yield is "high." If neither of these conditions are fulfilled, the correction terms must be evaluated quantitatively.

As to the reported periodic dependence of the x-ray production cross section of copper targets on the atomic number of the incident ion,[7] the inclusion of the corrections will *increase* the peak-to-valley ratio. The corrections (which are always negative) will have the largest effect on the smallest values of the cross sections.

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