14 Aug 1991

Binary Peak Enhancement And Structure In Partially Stripped Ion-atom Collisions

D. R. Schultz

Ronald E. Olson
Missouri University of Science and Technology, olson@mst.edu

Recommended Citation

D. R. Schultz and R. E. Olson, "Binary Peak Enhancement And Structure In Partially Stripped Ion-atom Collisions," *Journal of Physics B: Atomic, Molecular and Optical Physics*, vol. 24, no. 15, pp. 3409 - 3432, IOP Publishing, Aug 1991.
The definitive version is available at https://doi.org/10.1088/0953-4075/24/15/011

Journal of Physics B: Atomic, Molecular and Optical Physics

Binary peak enhancement and structure in partially stripped ion-atom collisions

To cite this article: D R Schultz and R E Olson 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 3409

J. Phys. B: At. Mol. Opt. Phys. **24** (1991) 3409-3432. Printed in the UK

Binary peak enhancement and structure in partially stripped ion–atom collisions

D R Schultz and R E Olson

Department of Physics and Laboratory for Atomic and Molecular Research, University of Missouri-Rolla, Rolla, MO 65401, USA

Received 18 March 1991, in final form 17 May 1991

Abstract. Recent experiments have found both an unexpected enhancement and structure of the binary peak in the spectrum of electrons ejected in partially stripped ion-atom collisions. Utilizing the theoretical approach which has been used to elucidate the origin of this behaviour, a survey of their manifestation is presented over a broad range of nuclear and ionic charges (C, F, Fe, I and U ions) and impact energies (0.1 to 100 MeV u^{-1}). For forward binary electron emission it is shown that the greatest enhancement occurs for the lowest projectile ion charge states (highly screened nuclei). The magnitude of the enhancement maximizes near an energy that is characteristic of each nuclear species and results in a cross section several times larger than that for impact by the fully stripped ion. Those ions, collision energies and ejection angles for which unusual binary peak structures are likely to be observable are illustrated. We point out what consequences these effects have for modelling energy deposition in the collision of ions with dense targets.

1. *Introduction*

For impact by bare ions, the binary peak in the spectrum of electrons ejected in energetic ion-atom collisions has been a thoroughly investigated phenomenon (Rudd and Jorgensen 1963, Rudd *et al* 1966, Bonsen and Vriens 1970, Stolterfoht *et al* 1974, Toburen and Wilson 1979, Stolterfoht 1978, Toburen *et al* 1980, Lee *et al* 1990) and its formation has in general been thought to be well understood. It has been found, for example, that at high collision energies the binary peak magnitude for impact by fully stripped ions scales as the square of the projectile's charge. Extension of the results of these experiments by scaling the cross sections for partially stripped ion impact by either the square of the projectile nuclear charge (Z) or its ionic charge (q), or by some value intermediate between these two extremes (Stolterfoht *et al* 1974, Stolterfoht 1978, Toburen and Wilson 1979, Toburen *et al* 1980, 1981) has met with some success. However, two recent experiments have dramatically illustrated that these proposed scalings are totally inadequate to explain the behaviour of the binary peak in partially stripped ion impact, and their results have, in fact, been termed 'anomalous'.

In the first of these, Kelbch *et al* (1989) found that at certain ejection angles, instead of the usual binary peak, an unexpected double peak structure appeared when a highly energetic (1.4 MeV u^{-1}) partially stripped uranium ion collided with a noble gas. In the second, Richard *et al* (1990), investigating the energy distribution of electrons ejected at 0° in the laboratory frame, observed that the impact of H_2 or He by the partially stripped ions of fluorine yielded greater binary peak magnitudes than did the bare fluorine ion, contrary to the predicted scaling. These anomalies present a

0953-4075/91/153409+24$03.50

fundamental challenge to theoretical explanation since, of the entire ejected electron spectrum in ion–atom collisions, the binary peak may be most readily modelled.

Furthermore, these new findings pose significant practical problems. For example, the binary peak is often used as a benchmark for the absolute normalization of the whole ionized electron spectrum since very simple models seemed adequate to predict its magnitude and position. Also, the binary electrons ejected in the collisions of ions impinging upon the atoms of a solid or biological material can be the largest source of damage in such collisions (e.g. Katz 1988). Consequently, models of important processes such as the radiation damage of human tissue and the effects of ion impact on semiconductor devices, which require reliable, accurate estimates of the ejected electron spectrum, could be substantially influenced.

As with many anomalies, the origin of this unexpected behaviour has a quite simple explanation which was only at first not apparent. The common link between the 0° enhancement and the non-0° peak structures observed is the fact that the target electrons are scattered by a partially stripped projectile which presents to them a strongly non-Coulomb potential, unlike in the case of a bare projectile. The 0° behaviour has been explained and quantitatively reproduced by Reinhold *et al* (1990) utilizing the binary encounter approximation modified for the case of model potential interactions. In addition, several other authors have made elastic scattering calculations to estimate the degree of enhancement for fluorine ion impact (Quinteros and Reading 1991, Shingal *et al* 1990, Taulbjerg 1990). The non-0° double peak structure has also been explained utilizing the modified binary encounter approximation of Reinhold *et al* (1991b).

Here we illustrate the range of ions and energies over which these effects should be expected to occur, in order to serve as a guide to experiment and to theory seeking to predict the magnitude and form of the binary peak for partially stripped ion impact. We present calculations for a number of species (C, F, Fe, I, U) spanning the range of nuclear and ionic charge states (e.g. F^{q+}, $q = 1, 4, 7$) and over a wide range of impact energies (0.1–100 MeV u^{-1}). The survey illustrates the magnitude of the enhancement at 0° expected for the binary peak when partially stripped ion impact is compared with bare ion impact. It is shown that the lowest charge states yield the greatest enhancements, which can reach a factor of several hundred per cent. We demonstrate that the energy at which this maximum enhancement occurs is similar for all ions of particular species and roughly follows a simple law. Further, elastic cross sections which indicate the origin of structures which should be expected in non-0° peaks, at least for the heavier ions, are presented.

Thus, we attempt to illustrate the nature of the enhancement and oscillatory structure for this wide range of collision systems. In particular, in section 2 we discuss the origin and formation of the binary peak and how its nature differs from the rest of the ejected electron spectrum. Section 3 is devoted to a brief outline of the theoretical method used and subsequent sections describe our survey of 0° enhancements (section 4) and non-0° behaviour (section 5). Finally, in section 6 we discuss the ramifications these results have on the modelling of ion–dense-target interactions.

2. Background

So-called binary electrons arise in very close collisions between a projectile and a target electron. In these collisions the target core, composed of the nucleus and the

other electrons, plays only the role of spectator. In fact, energy and momentum conservation yield the result that in the two-body collision of a projectile with an electron at rest, the electron obtains the energy E_b given by

$$E_b = 2m(\mu/m)^2 v^2 \cos^2\theta - U_i \tag{1}$$

where m is the mass of the electron, μ the reduced mass of the electron–projectile system, v the projectile velocity, θ the electron ejection angle and U_i is the energy (ionization potential) required to remove the electron from the atom. Since the electrons of the atom are not initially at rest but rather have a distribution of vector momenta, the binary electrons produced will have a distribution of ejection energies and angles. The peak of this distribution in energy will be at energies near, or slightly less than E_b. Shifts from this position are caused by the fact that the ejected electron escapes the collision region in the two-centre field of the residual target ion and projectile, affecting its final energy and angle, and by the fact that the electrons are polarized by the projectile charge prior to the collision. This latter effect can be very significant for highly-charged ion impact. In general, binary electrons are the most energetic electrons ionized from the target in ion–atom collisions. They form, therefore, a peak or shoulder at the high energy end of the spectrum of ejected electrons. Only in some cases for high-Z ion impact, electrons ejected from the projectile can produce ionized electrons with energies greater than that of the target binary peak (Olson *et al* 1990a) due to the broad Compton profile of the ion.

The entire spectrum, illustrated schematically in figure 1, is composed of a number of contributions. At the very highest ejection energy is the binary region. For large impact energies this region is characterized by a peak, but at lower impact energies or large ejection angles, the binary peak may merge with the rest of the spectrum and form only a shoulder or may not be observed as a distinguishable feature. For low ejection energies, the ionized electrons originate from distant, weaker collisions with the projectile, but in their escape, they interact strongly with the Coulomb fields of both the residual target ion and projectile. Thus, their distribution is more difficult to model in any simple way since a wide variety of geometries exists in both coordinate and momentum space. In general, one finds that the distribution is peaked near zero ejection energy and then declines as ejection energy increases. However, the decline is not without feature. For example, centred about an ejection energy corresponding to an electron velocity equal to projectile velocity, a cusp-like structure appears resulting from the focusing of ejected electrons into the continuum of the retreating projectile ion. Recent works (e.g. Reinhold *et al* 1987, Stolterfoht *et al* 1987, Olson *et al* 1987, Fainstein *et al* 1988a, b, Reinhold and Olson 1989, Brauner *et al* 1989, Reinhold *et al* 1990) have sought to identify and clarify the various, so-called two-centre effects, such as the cusp behaviour, and the saddle point electrons which have velocities about half that of the projectile. Finally, other features such as Auger peaks may be observed as well.

On the basis of rather simple ideas one can approximate the expected scaling of the electronic spectra on the magnitude of the projectile charge. Since the force between the electron and the projectile is proportional to Z, in the absence of other considerations, the cross section should scale as Z^2. This is just the scaling that the Bethe–Born theory of ionization yields. Departures from this scaling for the low and intermediate energy portions of the spectrum are well known. Moreover, since in the binary collisions the target electron passes very close to the projectile nucleus it might have been expected

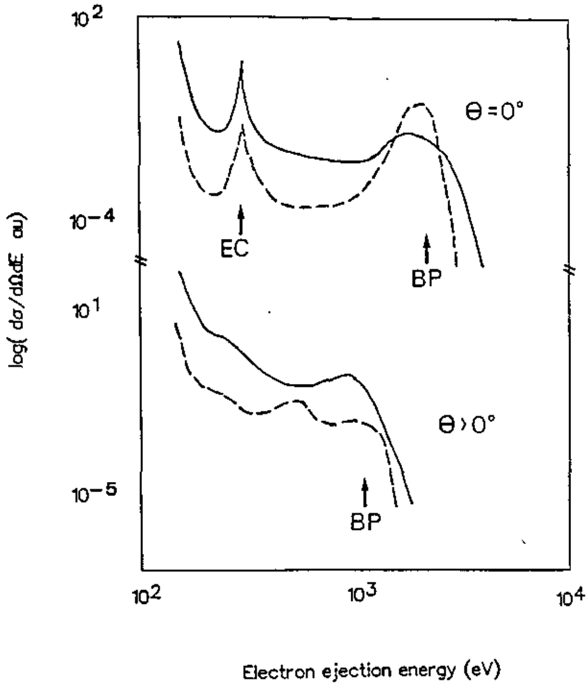

Figure 1. Schematic illustration of the enhancement and oscillation of the binary peak in the doubly differential spectrum of electrons ionized in partially stripped ion impact (broken curve), compared to the yield of electrons from fully stripped ion impact (full curve). The arrows indicate the electron cusp (EC), where projectile and electron velocities are equal, and the binary peak (BP) position predicted by equation (1). The scales represent units typical for impact by an ion such as Xe^{11+} at 1 MeV u^{-1} and for ejection angles of 0° and 30°.

that the binary peak should scale in this manner. Or, based on the success of various schemes of assigning effective charges (e.g. Slater's rules) which approximate the effects of screening produced by the presence of the other target electrons, the binary peak should scale by some factor between q^2, the square of the ionic charge, and Z^2. However, the new experiments show that this is not the case. Figure 1 also attempts to illustrate that in partially stripped ion impact the magnitude of the binary peak may exceed that produced by the bare ion, or, perhaps even more surprisingly, it may display a double peak structure at certain ejection angles.

The binary peak may be treated theoretically by any of the number of successful theories of ionization, but perhaps the most simple and illuminating approach is the impulse, or binary encounter, approximation. This approximation, originally proposed by Chew (1950) in the case of high energy neutron-deuteron scattering, has been utilized not only in nuclear physics but also extensively applied in ion-atom collisions, and is described in a number of texts (e.g. Goldberger and Watson 1964, Coleman 1969, McDowell and Coleman 1970). The essence of this approximation is the assumption that when the time of the collision between the incoming projectile and the target electron is short compared to the electronic orbital period, effects due to interactions between the electron and the rest of the atom may be neglected. The only role of the target nucleus is to determine the momentum distribution of the electron. The scattering

amplitude thus reduces from a many-body form to that for a two-body collision. Thus, in this view, the projectile provides an 'impulse' to the electron in the 'binary encounter'.

Regarding ion–atom collisions specifically, the binary encounter approximation was first introduced by Gryzinski (1959, 1965a, b, c) and subsequently applied and developed by a number of authors, including, notably, Gerjuoy (1966), Garcia *et al* (1968), Vriens (1969) and Bonsen and Vriens (1970). Within this approximation the ejected electron spectrum is simply given by the convolution of the cross section for elastic scattering of the target electron by the impinging ion and its momentum distribution. The binary peak may therefore be considered the quasi-elastic peak. The limits of integration in this convolution are given by energy and momentum conservation. The distribution of binary electrons in this approximation, given by the cross section for ejection into a given energy ($\mathrm{d}E$) and angular ($\mathrm{d}\Omega_{\mathrm{L}}$) range in the laboratory is

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}E\,\mathrm{d}\Omega_{\mathrm{L}}}=\int_0^{2\pi}\mathrm{d}\phi\int\mathrm{d}v_{\mathrm{e}}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}(\gamma)\frac{v_{\mathrm{e}}'}{v_{\mathrm{e}}}\rho(v_{\mathrm{e}}) \tag{2}$$

where v_{e} and v_{e}' are the initial and final electron velocities, $\rho(v_{\mathrm{e}})$ is the electronic momentum distribution, and Ω is the solid scattering angle in the projectile frame. The function γ relates the change in the relative velocity vector which defines the scattering angle (cf Reinhold *et al* 1991a, Bonsen and Vriens 1970).

If we consider the binary electrons produced from collisions of bare ions with a few-electron target, the result of the convolution of the elastic cross section with the electronic momentum distribution is that the binary peak is produced with a width that is proportional to the target momentum distribution or Compton profile. In these terms the zero degree enhancements of the binary peak observed by Richard *et al* (1990) are due to the fact that, for partially stripped ions, the elastic cross sections at backward angles in the projectile frame are larger for these ions than for the fully stripped ion, and lead to enhanced binary peaks in the forward direction in the laboratory frame. Further, if the elastic cross section is not smooth, but has significant structure or oscillation, the convolution will result in a binary electron distribution which may reflect these features. Thus, the double peak observed by Kelbch *et al* (1989) represents such a case where the elastic cross section has a deep minimum which survives the convolution.

We demonstrate a wide range of systems in which these heretofore anomalous features should be observable by presenting calculations of the elastic cross section for the scattering of an electron from a clothed projectile for a wide range of energies and ionic species. The magnitude of the enhancement of the binary peak may be found by simply considering the ratio of the elastic cross section to the Rutherford cross section, which closely represents the result for fully stripped ions, at the peak energy. This further has the advantage that the target ion is then not relevant since the momentum distribution which would distinguish it is not considered, the ratio pertaining only to the enhancement and not the details of the shape or form of the full peak. Similarly, the unusual structure which the binary peak should be expected to exhibit may be illustrated by showing in what species and energy range large oscillations of the elastic cross section can arise. In the section which follows we briefly summarize the method utilized to calculate the elastic differential cross section, the choice of model potential interactions and the transformation from projectile to laboratory frames.

3. Theoretical method

The calculation of the elastic differential cross section for the scattering of an electron in a potential is an elementary problem (see e.g. Joachain 1983, Rodberg and Thaler 1967), however a few complications arise. Under consideration is the scattering of an electron from an ion which is partially stripped. In this case the short range part of the interaction is non-Coulomb and the large range presents a Coulomb tail. The most common elementary derivations of the elastic cross section assume either a pure Coulomb potential or a non-Coulomb potential which is cut off at some small radius. Therefore, we briefly present here the essential features of the calculation for electron-partially stripped ion scattering. The radial Schrödinger equation containing the non-Coulomb interaction is solved numerically out to some large enough distance for each angular momentum of interest. At this so-called matching radius use is made of the known form for the phase shifts as a function of the radial wavefunction and its derivative. This also allows one to judge what angular momenta contribute significantly by observing the convergence of the phase shifts. The elastic differential cross section is then obtained from a properly weighted sum of the partial wave contributions to the amplitude.

The differential cross section for scattering into some solid angle range, $d\Omega$, as a function of scattering angle is

$$d\sigma/d\Omega = |f(\theta)|^2 \tag{3}$$

where the amplitude is composed of both a Coulomb and non-Coulomb part, i.e.

$$f(\theta) = f_C(\theta) + f_{nC}(\theta). \tag{4}$$

As is well known, the Coulomb phase shifts are given by

$$\sigma_l = \arg(\Gamma(l+1+i\alpha)) \tag{5}$$

where in this case of electron scattering the Coulomb factor, α, for a bare ion of charge Z, is

$$\alpha = -2Z/v \tag{6}$$

with v the relative velocity. (Atomic units, in which $\hbar = m_e = 1$, have been used here and will be used throughout.) Also, readily found is the Coulomb amplitude

$$f_C = \frac{-\alpha\, \exp(2i\sigma_0)}{4\mu v\, \sin^2(\theta/2)} \exp[-i(\alpha/2)\log(\sin^2(\theta/2))]. \tag{7}$$

This immediately yields for the Coulomb scattering cross section

$$\frac{d\sigma_C}{d\Omega} = \frac{Z^2}{16E^2 \sin^4(\theta/2)} \tag{8}$$

which is the well known Rutherford cross section. Thus, for bare ion impact, the binary encounter approximation gives a result which is the convolution of the Rutherford cross section, a smoothly varying function, with the target momentum distribution, and thus yields the shape usually observed.

For an arbitrary potential, there is of course no analytic solution and the Schrödinger equation must be solved by either approximation techniques or numerically. One may make a partial wave expansion for the non-Coulomb amplitude as

$$f_{nC}(\theta) = \frac{1}{2ik} \sum_{l\geq 0} (2l+1)\, e^{2i\sigma_l}(e^{2i\delta_l} - 1) P_l(\cos\theta) \tag{9}$$

where δ_l is the non-Coulomb phase shift. The radial Schrödinger equation is

$$u_l''(r)+(k^2+2\mu V-l(l+1)/r^2)u_l(r)=0 \tag{10}$$

where u_l is the radial wavefunction of angular momentum l and V is the potential. As in the present situation, if the potential is one in which a short-ranged part modifies the long-ranged Coulomb interaction, then the general solution of this hypergeometric differential equation behaves as

$$u_l(kr) \xrightarrow[r\to\infty]{} c_1F_l(\alpha, kr)+c_2G_l(\alpha, kr) \tag{11}$$

where F_l and G_l are regular and irregular solutions (cf Joachain 1983). It may be shown that the phase shift is found from

$$\tan\delta_l=c_2/c_1. \tag{12}$$

Defining the logarithmic derivative

$$L=u_l'/u_l \tag{13}$$

we have after a little algebra

$$\tan\delta_l=\frac{[(L/k)F_l-F_l']}{[G_l'-(L/k)G_l]}. \tag{14}$$

The condition that at some sufficiently large radius, $r_{\rm m}$, the wavefunction and its derivative must be continuous, allows one to integrate numerically the radial Schrödinger equation out to $r_{\rm m}$ finding u_l and u_l', and then use the form (14) to obtain the phase shift taking into account the asymptotic form of these radial functions through knowledge of the asymptotic form of the hypergeometric functions. Thus, in equation (11) α takes the value $2q/v$, where q is the asymptotic, ionic Coulomb charge. In this work we have used a numerical integration scheme (Johnson 1973) which utilizes the logarithmic derivatives, directly transforming the radial Schrödinger equation to the Ricatti equation. This has the benefit of an error term decreased by one power of the step size when compared to the Numerov method, and the fact that it is the logarithmic derivative which is the quantity that we wish to find.

The form of the potential used here is one which is parametrized in such a way that the large range of ionic species that we wish to consider may easily be accommodated. This potential is the Hartree–Fock model potential of Garvey *et al* (1975) which simulates the interparticle separation dependent screening of the ion nuclear charge experienced by the electron and is given by

$$V(r)=\frac{[(N-1)(1-\Omega(r))-Z]}{r} \tag{15a}$$

where

$$\Omega(r)=[(\eta/\xi)(e^{\xi r}-1)+1]^{-1} \tag{15b}$$

and where $(N-1)$ is the number of electrons present in the ion and the screening parameters, $\eta(Z, N)$ and $\xi(Z, N)$, have been tabulated for any ion with $2\leqslant Z\leqslant 54$. For heavier ions, the parameters may be found by a fit which utilizes points found from a reduced parameter form of this potential by the same group (Green *et al* 1969). We neglect the polarization of the ion electronic cloud since the effects which cause the anomalous behaviour stem from small to intermediate impact parameters and will

be influenced very little by polarization. In addition, previous calculations (Reinhold *et al* 1990, 1991a) utilizing this potential have given excellent agreement with the measurements of Richard *et al* (1990) for the binary peaks in $F^{q+} + H_2$ and He.

Also neglected in this calculation is the effect of electron exchange. That is, since the target electron is indistinguishable from the electrons of the ion from which it scatters, an amplitude should be introduced to account for exchange. Taulbjerg (1990) has considered exchange in a one electron ion (F^{8+}) colliding with H_2 and He and has found that exchange contributes about ten per cent to the enhancement of the binary peak. In this survey, however, we will often be concerned with partially stripped ions with many electrons; consequently, some mention should be made as to the expected effects of exchange.

The calculation of the exchange amplitude when many electrons are present is a difficult task. It is, however, possible to estimate how many electrons would contribute. Since the probability of exchange decreases with increasing relative collision velocity, we may note that only the electrons within a shell with orbital velocities which, when added to the collision velocity, yield small relative velocities to the target electron and thus produce a strong overlap in the exchange amplitude, will contribute significantly. Thus, the maximum influence of exchange could be several times as large as the one-electron result if the individual amplitudes added coherently. However, it would not be expected that all the individual amplitudes for those 'active' electrons would sum coherently, and effects of spin and scattering angle dependence would also have to be accounted for. We therefore estimate that over the wide range of ions that we consider here, exchange could amount to at least a ten per cent modification, and possibly a factor of several times that amount for ions with many electrons. Clearly, future investigations should consider in detail the difficult task of calculating the influence of exchange quantitatively.

Two other possible considerations bear mention as well. When the impinging ions are of large atomic number, spin–orbit effects in the scattering of the target electron may play a role. In particular, depending on the spin projection of the electron, the spin–orbit interaction would either make the potential more attractive or repulsive, as demonstrated by the Mott scattering of electrons from heavy atoms (see e.g. Kessler 1985). However, in collision systems with many electrons, it is expected that these effects more or less cancel. Calculations neglecting the spin–orbit potential have already been shown to give good agreement with experiments showing the unusual binary peak structure in $U^{21+} + He$ collisions (Reinhold *et al* 1991b).

The second is the effect of relativity. We note that the innermost shells of heavy ions are significantly influenced by the relativistic motion of the electrons. These relativistic effects influence the inner shell wavefunctions and thereby the form of the potential which represents their screening of the nucleus. Therefore, potentials which represent a more detailed treatment of inner shells would be a useful extension of the present investigation. However, a general, easy to implement form for such a more elaborated potential does not seem to be readily available. We have found that small changes to the potential that we employ do not drastically alter the elastic cross sections. Further, ejected electron spectra calculated using non-relativistic methods (classical trajectory Monte Carlo) are in good agreement with experiments using U^{91+} and U^{92+} projectiles at 120 and 420 MeV u^{-1} (Berg *et al* 1988).

Finally, since in what follows we describe effects in both the projectile and laboratory frames of reference, we indicate the relation of these two frames as concerns the binary peak. If we consider the x–z plane as the scattering plane then the electron velocity

components in the projectile frame is given by

$$v_{p_x} = v_t \sin\theta_t \qquad v_{p_z} = v_t \cos\theta_t - v_p \tag{16}$$

where the subscripts p and t refer to the projectile and target frames, respectively. From these one readily defines the scattering angle

$$\cos\theta_p = -v_{p_z}/(v_{p_x}^2 + v_{p_z}^2)^{1/2}. \tag{17}$$

Substitution of the relations (16) in equation (17) yields a form which cannot be further simplified. But, we note that at the binary peak

$$v_t \simeq 2v_p \cos\theta_t \tag{18}$$

which may be seen from equation (1) taking the reduced mass to be equal to one and neglecting the binding energy term. With this approximation (17) becomes, after some rearrangement of terms,

$$\cos\theta_p = 1 - 2\cos^2\theta_t \tag{19}$$

or, taking advantage of well known trigonometric relations,

$$\theta_p = \pi - 2\theta_t. \tag{20}$$

This expression is, of course, only valid at the binary peak, and there only approximately, but it does give a useful rule of thumb to relate features of the elastic cross section for the scattering of the target electron by the projectile to what result occurs in the laboratory. For example, one sees from this expression that if we consider binary electrons ejected at zero degrees in the laboratory, this corresponds to scattering by 180°, direct backscattering, in the projectile frame.

4. Forward angle behaviour

The relationship that backward scattering in the projectile frame corresponds to forward ejection in the laboratory allows us to survey the enhancement of the zero-degree binary peak. This is presented as the ratio of the elastic cross section for scattering by 180°, which we obtained in our partial wave solution to the Schrödinger equation for an electron colliding with a partially stripped ion, and the Rutherford cross section at 180° for the bare ion. This ratio represents the relative magnitude of the binary peak for the partially stripped ion compared with that for the fully stripped ion, evaluated at the maximum of the binary peak. Thus, the behaviour is illustrated without recourse to the more elaborate and costly impulse approximation which would reflect the shape and magnitude of the entire binary peak more fully.

In figures 2 through 6 we present the results of such calculations for a wide range of nuclear species (C, F, Fe, I and U ions) and over the range of charge states possible with these ions, as a function of collision energy. Inspection of these figures indicates that an enhancement of the forward binary peak for partially stripped ion impact exists over a broad range of systems. Also immediately noted is the fact that the enhancement reaches its largest value when the ratio of ionic charge to nuclear charge (q/Z) is smallest. The maximum enhancement for a particular nuclear species comes for the lowest charge state. For example, Fe^{2+} produces a larger maximum enhancement than does Fe^{11+}. Likewise, the effect for U^{2+} ($q/Z = 0.022$) has a greater maximum than Fe^{2+} ($q/Z = 0.077$).

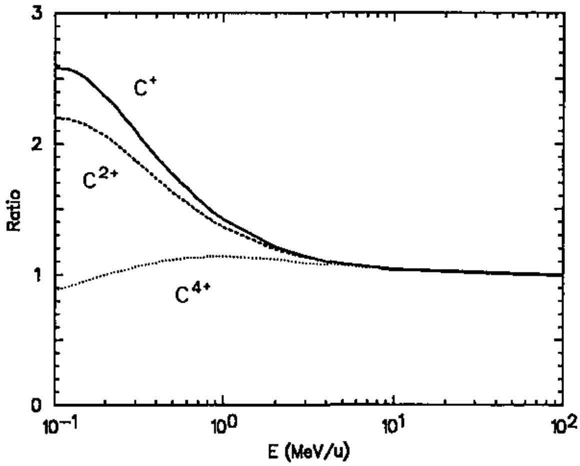

Figure 2. Ratio of the elastic scattering cross section for a target electron colliding with various partially stripped carbon ions (C^{q+}, $q = 1, 2, 4$, $Z = 6$) to that for the fully stripped ion at 180° in the projectile frame. As explained in the text, this corresponds to the ratio of the binary electron yields at 0° in the laboratory frame.

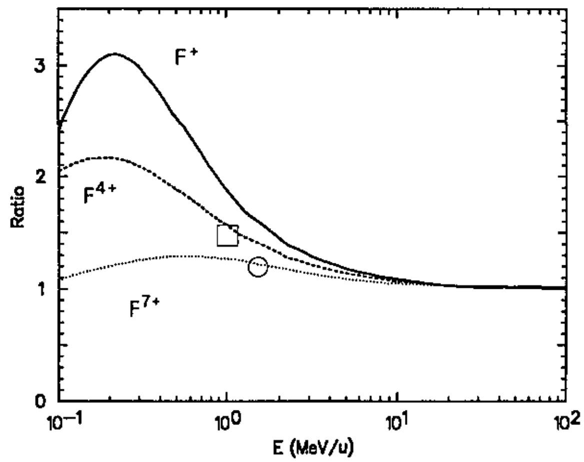

Figure 3. Same as figure 2 except for fluorine ions (F^{q+}, $q = 1, 4, 7$, $Z = 9$). The points represent the experimental measurements of this ratio by Richard *et al* (1990) for F^{4+} at 1 MeV u^{-1} and F^{7+} at 1.5 MeV u^{-1} colliding with H_2.

Further, the increase in binary electron production for the partially stripped ions related to that for bare ion impact is not a constant function of the impact energy. At large impact energies the ratio of these productions tends to one, implying that the Z^2 scaling is valid in that regime, and at low energy it drops below one, approaching the q^2 scaling of the cross sections. We should note that at very low energies, the binary peak may not be a distinct feature of the ejected electron spectrum, being subsumed into the intermediate energy electron distribution. However, the ratio presented still reflects the relative production rates of binary electrons, even if the binary peaks are not separately distinguishable.

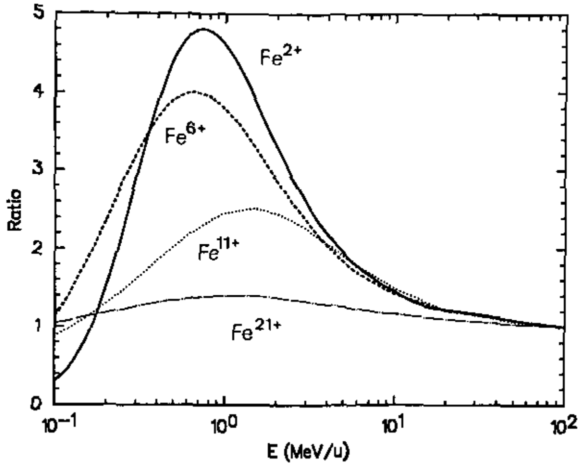

Figure 4. Same as figure 2 except for iron ions (Fe^{q+}, $q=2, 6, 11, 21$, $Z=26$).

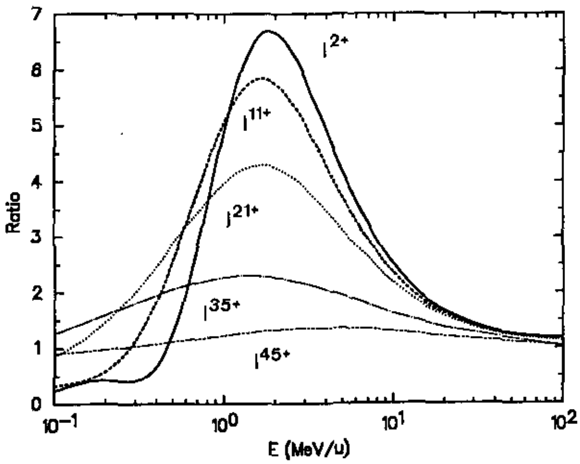

Figure 5. Same as figure 2 except for iodine ions (I^{q+}, $q=2$, 11, 21, 35, 45, $Z=53$).

In the intermediate range of impact energies the greatest enhancements occur. For light ions such as carbon or fluorine this occurs at a few hundred keV u^{-1} and the low charge state ions display binary peak magnitudes two to three times as large as those for bare ions. The maximum is found at energies of a few MeV u^{-1} and the enhancements can reach factors of five to nine for the lowest charge states, for the heavy ions. In fact, the maximum of the enhancement occurs within a relatively narrow energy range for each ionic charge state of a given nuclear species. Thus, for example, all uranium ions have the greatest effect at about 4 MeV u^{-1}. This rule is not strict, and variations from this peak position occur, especially for the highest charge states where the maximum moves to higher energies.

At the energy where the maximum occurs, the enhancements are quite strictly ordered in terms of the q/Z ratio, but, especially in the energy range just below the maximum, the orderings are not so conveniently arranged. For example, the low charge states have a quite steep rise to the maximum as a function of energy, whereas the

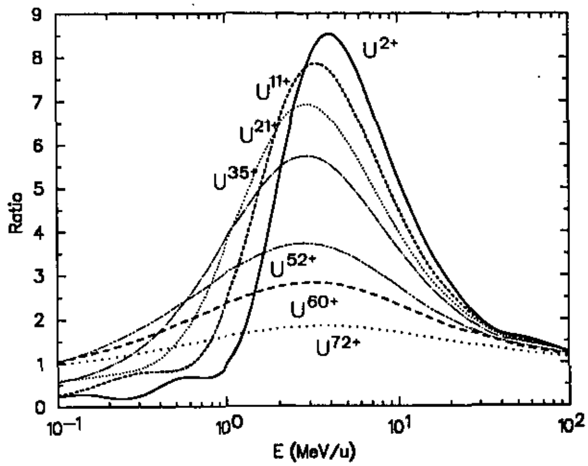

Figure 6. Same as figure 2 except for uranium ions (U^{q+}, $q = 2, 11, 21, 35, 52, 60, 72, Z = 92$).

high charge states have a slower rise and display a much broader distribution about the maximum. Consequently, experiments to measure the magnitude of the enhancement would find that which ion charge state produced the greatest binary peak would be dependent on impact energy.

But what is the origin of this behaviour? The most straightforward and concise explanation is that the elastic scattering of the target electron by the projectile is modified by the presence of the non-Coulomb interaction, arising because the electrons of the partially stripped ion screen the nuclear charge. Thus the quasi-elastic, binary peak is modified. This is, of course, the cause, but what is the mechanism? To answer this Reinhold *et al* (1990, 1991a) looked to the classical deflection function, that is, the relation in classical potential scattering between the scattering angle and the impact parameter.

The classical elastic differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \frac{1}{\sin\theta} \sum_i b_i \left| \frac{db_j}{d\Theta(b)} \right| \tag{21}$$

where θ is the scattering angle, b the impact parameter, i indexes the various branches of the deflection function, Θ is the deflection function and the sum extends over all impact parameters which lead to scattering to a single angle (cf McDowell and Coleman 1970). As has been widely noted, this relation is what leads to the great variety of phenomena possible in classical potential scattering, since Θ or its derivative with respect to b may possess singularities, or since different branches of Θ may superpose due to the sum. The deflection function is given by

$$\Theta(b) = \pi - 2b \int_{r_0}^{\infty} \frac{dr}{r^2} \left(1 - \frac{V(r)}{E} - \frac{b^2}{r^2} \right)^{-1/2} \tag{22}$$

where r_0 is the distance of closest approach, found as the root of the function

$$\left(1 - \frac{V(r)}{E} - \frac{b^2}{r^2} \right) \tag{23}$$

where r is the radial coordinate, $V(r)$ a central potential and E the collision energy. For scattering from a bare ion, the potential is simply the Coulomb potential and one

may analytically perform the integral in (22) and find that the relation (21) yields the Rutherford cross section. Thus, either classically or quantum mechanically the same result is obtained for scattering from the bare ion. The deflection function in this case, varies smoothly between zero and 180° as a function of impact parameter.

However, scattering from the non-Coulomb potential which models the screening present for the partially stripped ion, yields a much different behaviour. In fact, Reinhold *et al* (1990, 1991) found that the deflection function in this case may exceed 180°, leading to the phenomenon known as glory scattering, and possess a local minimum, resulting in rainbow effects (cf Ford and Wheeler 1959). These features of the deflection function are illustrated for electron scattering from the potential representing Fe^{11+}, for example, in figure 7 and for a stronger non-Coulomb case, U^{11+}, in figure 8. Whereas rainbow and glory scattering are well known in low energy atom–atom collisions (see e.g. Bernstein 1966) where both long range attractive and short range repulsive portions of the interaction exist, they are unexpected in the case of intermediate energy ion–atom collisions. The effect of the screening of the nuclear charge in the partially stripped ion case is to lower the velocity at which the electron reaches the distance of closest approach, allowing a greater time for deflection and the possibility that much larger impact parameters can contribute to a particular range of scattering angles, especially in the backward direction. Hence, the larger elastic cross section for the partially stripped ions at backward angles in the projectile frame, maps into an enhanced binary peak in the forward direction in the laboratory.

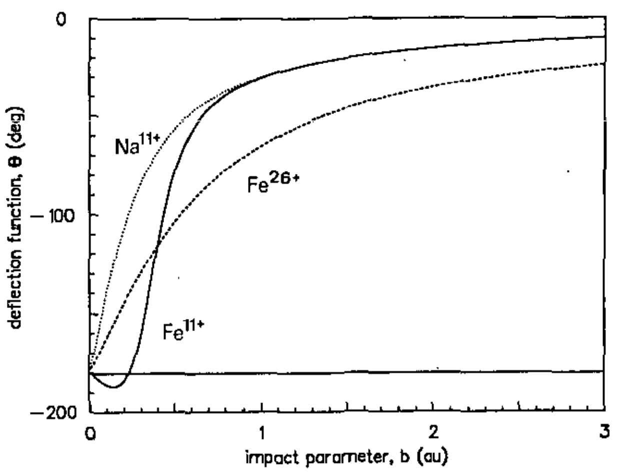

Figure 7. The classical deflection angle as a function of impact parameter for the elastic scattering of an electron from the partially stripped ion Fe^{11+} (full curve) compared with that for the bare ions of equal nuclear charge, Fe^{26+} (broken curve) and ionic charge, Na^{11+} (dotted curve) at 1 MeV u^{-1}. The horizontal line indicates 180°.

We may see this from an early model due to Lindhard (1976) and recalled by Quinteros and Reading (1991). If we consider a potential with Yukawa screening representing the interaction of an electron with a clothed ion and given by the form

$$V = -Z/r\, e^{-ar} \tag{24}$$

then upon expanding the exponential we have for $r \to 0$

$$V \approx -Z/r + Za. \tag{25}$$

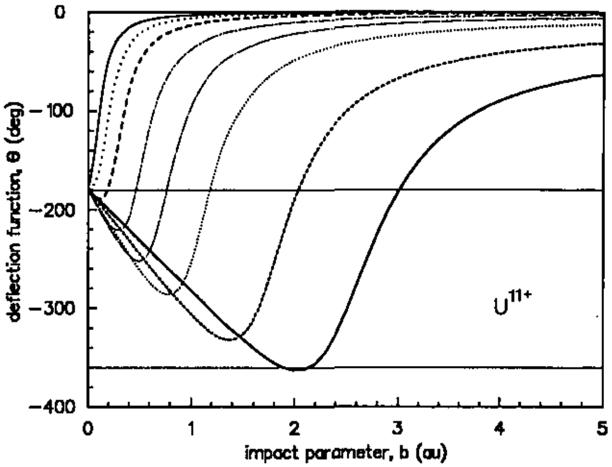

Figure 8. The same as figure 7 except for electron scattering from U^{11+} at various energies. The lowest curve is for 0.1 MeV u^{-1} and those above it are for 0.2, 0.5, 1, 2, 5, 10 and 20 MeV u^{-1}. Here the horizontal lines indicate 180° and 360°.

As Quinteros and Reading point out, the effect is to subtract a constant term from the energy in the Schrödinger equation, slowing the electron and increasing the Rutherford cross section since it varies inversely with the square of the energy. However, we may take this idea one step further. If we rearrange (22) and use the relation between angular momentum and impact parameter

$$b = l(l+1)/\mu v \tag{26}$$

we have

$$\Theta(b) = \pi - 2b \int_{r_0}^{\infty} \frac{E^{1/2}}{r^2}\left(E - V(r) - \frac{(l(l+1))^2}{2\mu r}\right)^{-1/2}. \tag{27}$$

Inserting the expanded form (25) into this we obtain for the term in parentheses

$$\left(E + \frac{Z}{r} - Za - \frac{(l(l+1))^2}{2\mu r^2}\right)^{-1/2}. \tag{28}$$

Since the greatest part of the deflection occurs at the distance of closest approach, the terms which are a function of r contribute a constant amount there, K, and we have

$$(E - Za + K)^{-1/2}. \tag{29}$$

Thus, in equation (8), if this effective energy, $E_{\text{eff}} = E - Za$, were used in place of E, the Rutherford cross section would become very large as $E - Za$ tended toward zero. A fit to the form (24) of the potentials utilized in this work for distances near the turning point, indicates that the screening constants take the value $a \approx 5$. In the spirit of this approximation, one could assume that there will be a peak in the enhancement relative to the bare charge that can be parametrized as a linear function of the projectile nuclear charge.

Indeed, the present calculations show that the results for each ion of a particular nuclear species peak near a single impact energy characteristic of that Z. For example,

the uranium ions, with $Z=92$ corresponding to $E=Z$ au of about 4.6 MeV u^{-1} (i.e. $E=92\ \mathrm{au}\times 27.2\ \mathrm{eV\,au}^{-1}\times 1836\ \mathrm{u}^{-1}=4.6\ \mathrm{MeV\,u}^{-1}$), have maxima at around 3 to 4 MeV u^{-1}. From the calculations we find that a good rule of thumb is that the maximum of the ratio of the partially stripped ion induced binary peak to that for the bare projectile occurs at around

$$E_{\max}\simeq 0.75\,Z. \tag{30}$$

The constant 0.75 is far from the value $a\simeq 5$ derived from the potentials, which further indicates the importance of the rainbow and glory interference effects in determining the backward enhancement ratio. We point out that the simple argument leading to this parametrization does not apply to energies below the peak since in that case $E-Za$ would be negative and the expression would be complex.

Also, at this energy where the maximum enhancement occurs, one may readily establish from the calculations that the ratio is

$$R(E_{\max})\approx\sqrt{Z}-q/\sqrt{Z}. \tag{31}$$

This parametrization was found by considering a straight line fit to a plot of the magnitude of the ratio at its maximum against ionic charge state. We note that since exchange has been estimated to increase the predicted enhancement on the order of 10–20% per cent for the one-electron ion F^{8+}, and since only a few electrons on the projectile will have orbital velocities in the range in which exchange should be significant, $R(E_{\max})$ could be multiplied by a factor $N=1+0.1(n_e)$ where n_e is the number of electrons within the appropriate shell.

Worthy of note is that at low impact energies the partially stripped ions produce fewer binary electrons than equivelocity bare ions, but that for the very lowest q/Z ions, glory oscillations in the energy dependence of the ratio of peak magnitudes are observed theoretically. The energy regime is sufficiently low that the binary peak will not be a distinguishable feature in the ionized electron distribution, however. Such oscillations have been studied in the case of low energy atom–atom scattering, as have been a number of other features of the behaviour noted here (see, for example, Child 1974).

In summary, at higher energies, the binary peak magnitude for partially stripped ion impact exceeds that produced by the bare ion, due to the glory created by the screening of the projectile nuclear charge experience by the target electron. The figures 2–6 presented illustrate the degree of this enhancement in the ratio and its behaviour and demonstrate the untenability of any proposed q^2 or Z^2 scaling. At very high energies, the effects of the difference between the scattering in either a Coulomb or screened potential diminish in importance and the asymptotic ratio of the binary peak magnitudes is one.

5. Non-zero degree effects

At ejection angles larger than zero degrees, the binary electrons are affected to a larger extent by the influence of the two-centre field created by the target and projectile ions and due to the $\cos^2\theta$ dependence of E_b the binary peak is found at lower energies. The result is that the binary peak merges more with the rest of the spectrum and is less clearly defined as a separate peak. Also, projectile electron loss may contribute to the observed spectrum. Therefore, estimates of the ratio of the binary peak magnitudes made using the technique above must be taken to indicate the relative formation rate

of binary electrons, rather than strictly the ratio of the heights of the peaks formed by either partially stripped or bare ions. With this caution, we consider in this section the behaviour of this ratio for angles larger than zero degrees. In addition, as has been demonstrated by Reinhold *et al* (1991b) and Schultz *et al* (1991), unusual structure in the binary peak region exists due to the quantum interference structures in the elastic scattering cross section. Therefore we survey here the elastic cross section as a function of impact energy to illustrate in what systems the oscillations are strong enough that they should survive the convolution over target electronic momentum to be present in the electronic spectrum.

First, we consider the behaviour of the ratio of the predicted binary peak magnitudes for a case in which we do not find any unusual oscillations in the elastic differential cross section. For this purpose, in figure 9 we display the ratio as a function of projectile charge state for carbon ions at an impact energy of 1 MeV u^{-1}. At the forward angles considered, 0°, 10° and 20°, the same pattern that we have discussed above is observed where the lowest charge states produce the largest enhancement over the bare ion result. The ratio declines with increasing charge state and approaches the value of one, indicating that the forward binary peaks for the partially stripped ions are at least as large as that produced by the bare ion even to the highest charge states.

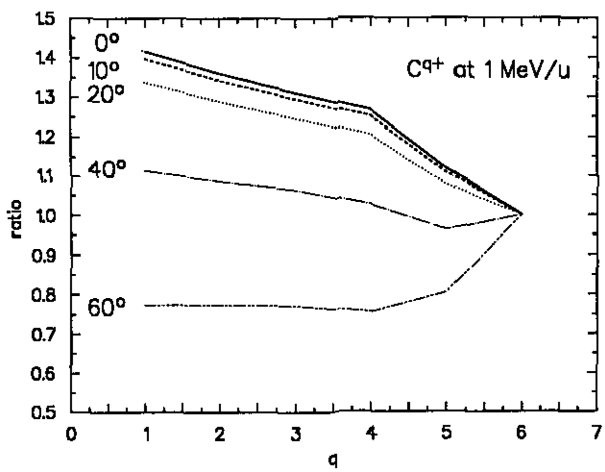

Figure 9. Predicted ratio of the binary peak magnitude for impact at 1 MeV u^{-1} by partially stripped carbon ions to that by the bare ion as a function of projectile charge state, for several ejection angles.

At larger ejection angles, such as 40° or 60°, the behaviour is not the same. In these cases the distance of closest approach between the target electron and the projectile nucleus is not as small as when zero-degree ejection occurs and the effect which leads to enhancement is therefore not as great. Consequently, for large ejection angles the ratio is much smaller and the binary electron production from the partially stripped ions may become less than that for the bare ion. However, this does not necessarily imply that there is no enhancement of binary peak over what one would obtain using a q^2 scaling. That is, even though the enhancement does not exceed a factor of Z^2, it may still exceed a factor of q^2, as has been recently shown experimentally by Jagutzki *et al* (1991).

The trend of this behaviour may also be seen directly from the elastic differential cross section. For the C^{2+} ion this is displayed in figure 10 for 0.1, 0.5 and 1 MeV u^{-1} collision energy. The full curve, which represents the elastic cross section for the scattering of a target electron by C^{2+} is seen to be larger than that for scattering from the bare C^{6+} ion, indicated by the dotted curve, at large projectile angles. These angles correspond to the forward direction in the laboratory frame and indicate the range of ejection angles over which the partially stripped ion's binary electron production should exceed the bare ion's. For 1 MeV u^{-1}, one sees that these two curves intersect at about 90°. Using equation (16) which relates angles in the projectile and laboratory frames, we see that this corresponds to a laboratory ejection angle of about 45°, consistent with what one would read from the previous figure as to where the C^{2+} and the C^{6+} ions should have the same binary electron production. Judging from the slope of these

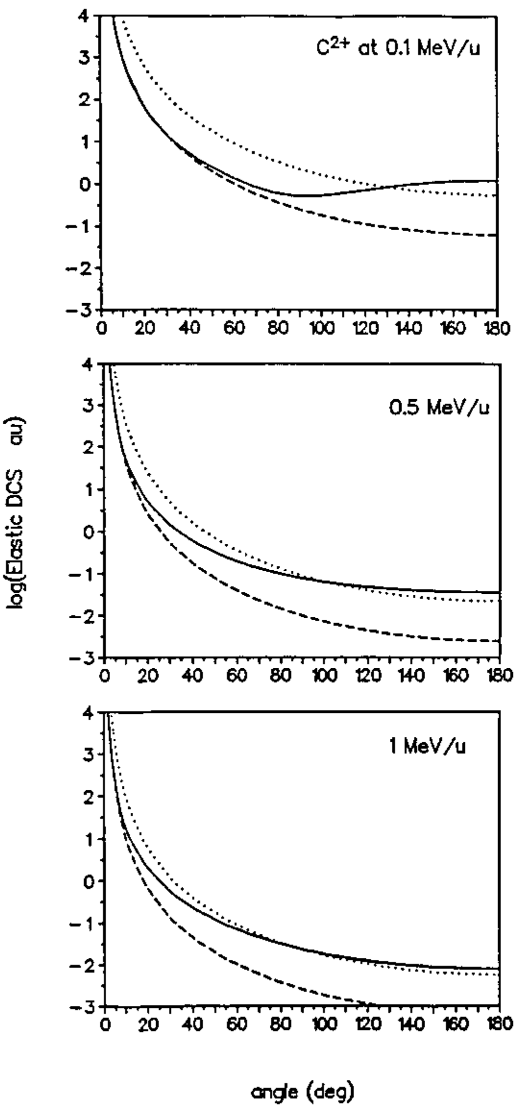

Figure 10. The elastic cross section in the projectile frame for scattering of a target electron by an impinging carbon ion. The figure compares this cross section for the partially stripped ion C^{2+} (full curves) to that for the fully stripped ion C^{6+} (dotted curves) and to that for a bare ion of nuclear charge equal to the ionic charge 2, He^{2+} (broken curves), at collision energies as indicated.

curves at backward projectile frame angles, we can also see that between 140° and 180° the enhancement of the C^{2+} cross section is roughly constant so that in the range of 0° to 20° in the laboratory the binary peak ratios should be roughly the same. For larger laboratory angles, the C^{2+} induced binary electron production decreases and goes below that for the bare ion.

Figures 11-14 display the elastic cross sections for particular ionic charge states of fluorine (F^+), iron (Fe^{11+}), iodine (I^{21+}) and uranium (U^{11+}), each for several collision energies, to illustrate the dependence of the cross section on E, Z and q. The full curves indicate the result of the quantum mechanical calculation utilizing the model potential for the partially stripped ions, the dotted curves represent the result for the bare ion of nuclear charge equal to that of the projectile ion and the broken curves are for a bare ion of nuclear charge equal to the ionic charge of the projectile. Thus, the figures compare the partially stripped ion result to scalings by either Z^2 or q^2. From them one can get an idea of the ejection angle range over which the partially stripped ion binary electron production should exceed the bare ion's, be roughly equal to it or lie between the Z^2 and q^2 results. For example, figure 11, for the F^+ ion, indicates that the largest enhancement of the binary peak should occur for the lowest collision energies displayed, but should be confined to the forward direction in the laboratory. In this case, the binary electron production relative to the bare ion result should fairly quickly decrease as laboratory angle increases. On the other hand, at higher impact energies, while the enhancement is much less, it should persist to much larger angles. At the highest energies, the ratio of partially stripped to bare ion binary electron production should of course reach one as noted above, and that the angular range in which the ratio is about one should be quite large.

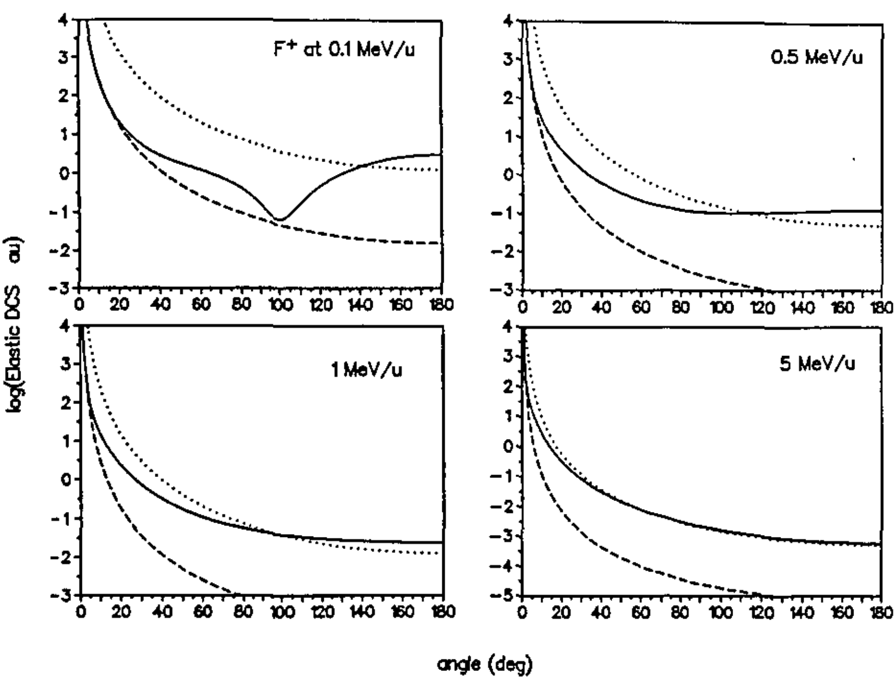

Figure 11. Same as figure 10 except for fluorine ions. The figure compares the elastic cross section for F^+ to that for the fully stripped ions of equal nuclear (F^{9+}) and ionic (H^+) charge.

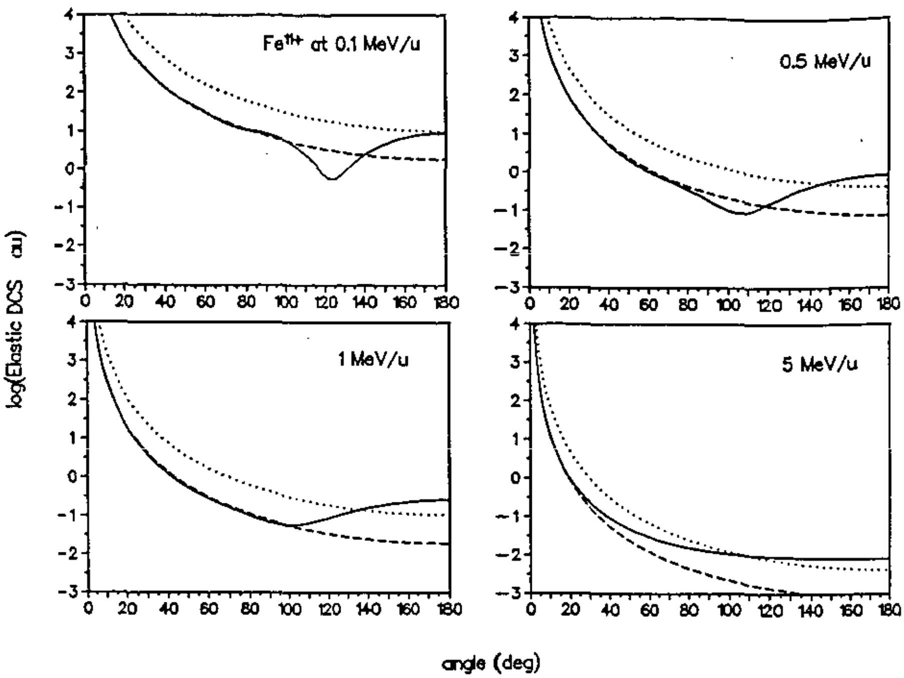

Figure 12. Same as figure 10 except for iron ions, comparing the elastic cross section for Fe^{11+} impact to that for the fully stripped ions of equal nuclear (Fe^{26+}) and ionic (Na^{11+}) charge.

Also immediately discernible from these figures is the fact that as the projectile nuclear charge increases, and therefore the available q/Z ratio may decrease, the presence of a great deal of structure of the elastic cross section become prevalent at the lower impact energies. If the minima of the structures are deep enough they may survive the convolution over target momentum and be observable in the electronic spectrum near where the binary peak would be predicted to appear according to equation (1). The case for which we have previously performed the full binary encounter treatment (Reinhold *et al* 1991b) to reproduce the experimentally observed double peak structure is most like that seen in figure 14 for U^{11+} at 1 MeV u^{-1}. The intriguing possibility of observing even more structure is evident from the behaviour displayed for lower collision energies and lower charge states of uranium. Certainly, this type of structure should exist for other heavy ions such as iodine as illustrated by figure 13.

Thus, the present survey indicates that for low charge states of intermediate energy heavy ions, a great deal of unusual structure should be observable at emission angles corresponding to the deep minima in the differential elastic cross section. We note that the magnitude and frequency of the oscillations of the elastic cross section increase with decreasing impact energy, but that at these lower impact energies, the binary region of the ejected electron spectrum becomes more blended with the lower ejection energy portions and consequently the most dramatic structures would probably be subsumed into the background. Also, it is important to emphasize that to facilitate observation of this type of unusual behaviour, that is, to make the structure as cleanly visible as possible, targets with the most narrow possible momentum distributions (e.g. H, H_2, He) should be utilized. The more narrow the target momentum distribution,

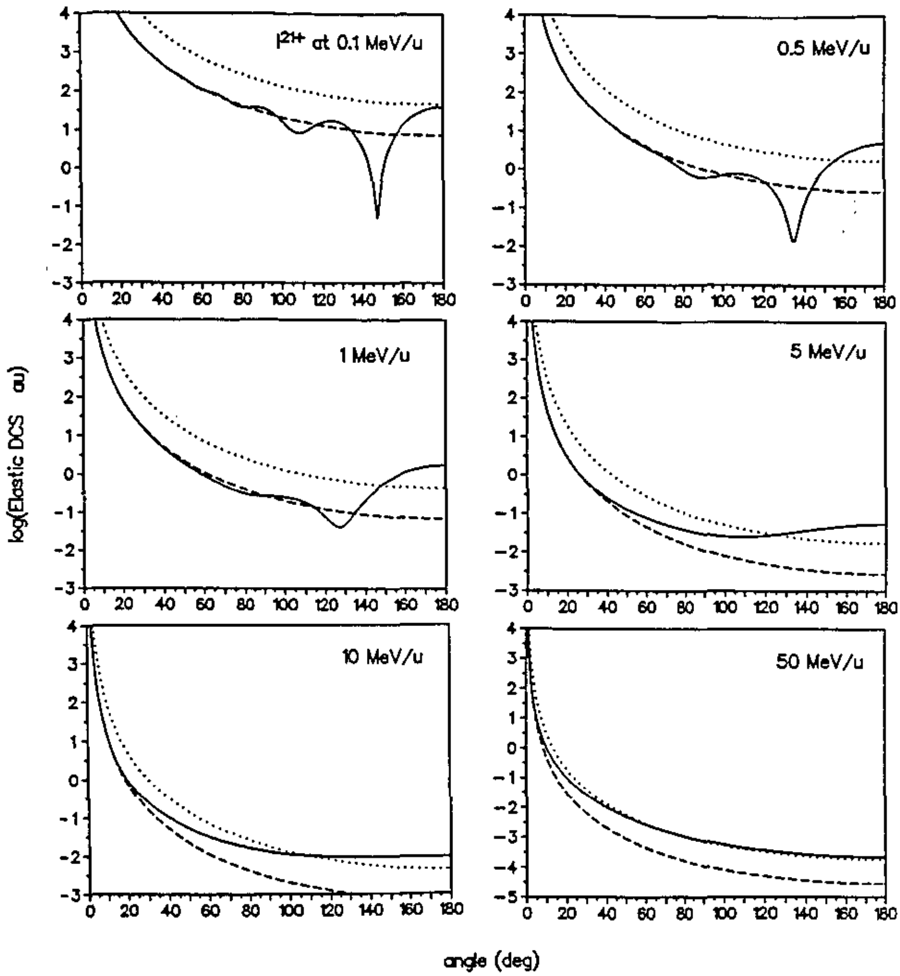

Figure 13. Same as figure 10 except for iodine ions, comparing the elastic cross section for I^{21+} impact to that for the fully stripped ions of equal nuclear (I^{56+}) and ionic (Sc^{21+}) charge.

the more sharply the rapid oscillations of the elastic cross section will be preserved in the convolution which takes place in theory as well as occurring physically.

We note that similar enhancements and oscillations should also be present in the spectrum of electrons lost from the projectile due to the analogous scattering of these electrons from the screened target atom and have been observed by Duncan and Menendez (1981) in the collisions of H^-, H_2^+ and He^+ at 0.5 MeV u^{-1} with Kr. Theoretical investigations along these lines are being undertaken by Wang *et al* (1991).

6. Ramifications in ion–dense-target modelling

Since the use of q^2 and Z^2 scalings prevails, we wish to emphasize that the unexpected behaviour which we have described here can have significant impact on the modelling

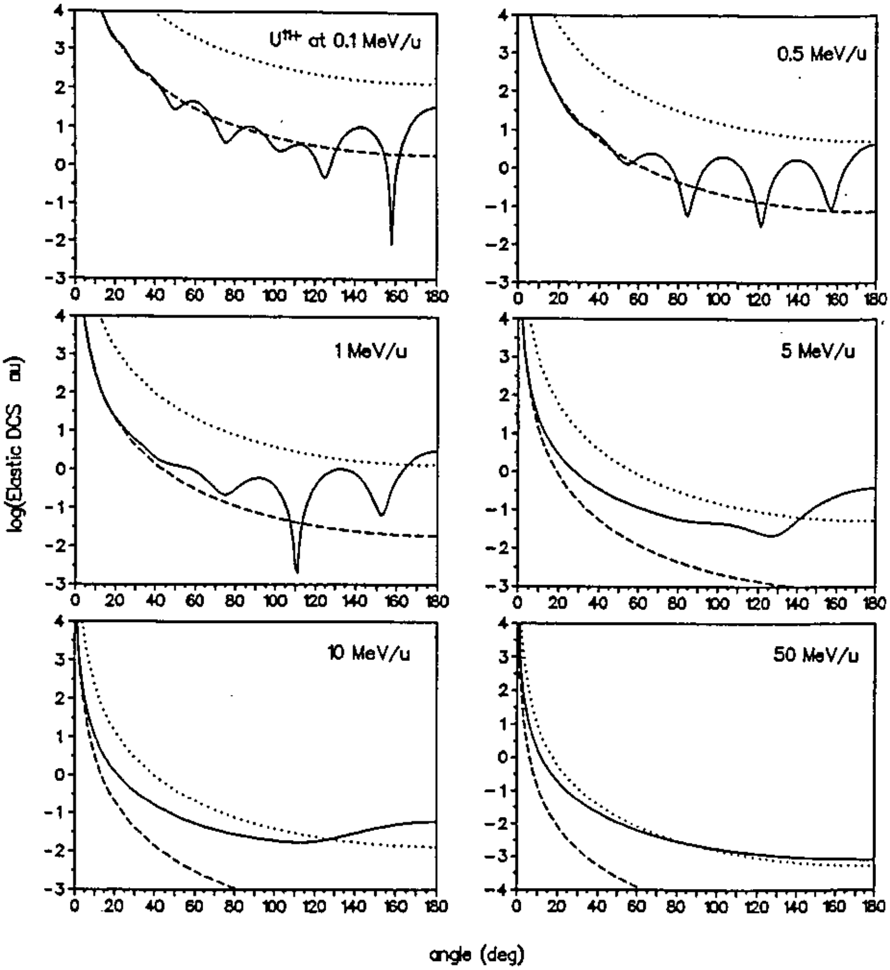

Figure 14. Same as figure 10 except for uranium ions, comparing the elastic cross section for U^{11+} impact to that for the fully stripped ions of equal nuclear (U^{92+}) and ionic (Sc^{11+}) charge.

of ion–dense-target collisions. One of the largest sources of damage in such collisions is the binary electrons, since they are very energetic and produced with large cross sections. Consequently, partially stripped ions, which have now been thoroughly demonstrated to yield binary electrons in quantities exceeding even bare ions of equal nuclear charge, are poorly modelled if the fully stripped ion impact data are simply scaled. These considerations are especially pertinent to a number of current, important studies including radiotherapy using heavy ions (e.g. Toburen *et al* 1989), biological effects of both naturally occurring and man-made radiation on human tissue (e.g. Katz 1989, Kraft 1987) and the hardening of space-borne semiconductors against cosmic, or man-made, nuclear radiation (e.g. Dressendorfer 1989, Price and Cross 1989).

Beyond simply stating that the newly described effects should be considered, a direct calculation will demonstrate the order of magnitude of their influence. Using

the classical trajectory Monte Carlo (CTMC) technique, previous works had demonstrated that the enhancement of the binary peak due to non-Coulomb scattering was present in the case of classical scattering of the target electrons from the projectile ion when a model potential was used. In fact, Olson *et al* (1990b) showed that the CTMC method yielded enhancements in the binary peak for partially stripped uranium ions colliding at 1.4 MeV u^{-1} with argon and, further, Jagutzki *et al* (1991) showed reasonable agreement between similar calculations and the experimental measurements of the ejeced electron spectrum in 0.53 MeV u^{-1} copper ions colliding with He.

The CTMC results indicated the presence of rainbow and glory effects, but compared with the same features calculated quantum mechanically, appeared to be overestimated. That is, the classical rainbow and glory singularities are stronger and lead typically to a cross section about a factor of two too large. The result is that the CTMC calculations give the correct behaviour of the enhancement, but not the corrected detailed form. While based on classical scattering, the CTMC results do include two-centre effects and the contributions of the low energy, non-binary electrons ejected in the collision, and thus provide an important treatment of the entire ionized electron distribution. In fact, CTMC calculations (Olson 1989) have been shown to provide excellent agreement with tabulated stopping powers.

In the present work, we calculated the stopping power for 1.4 MeV u^{-1} U^{29+} in neon with and without a model potential representing the projectile–electron interaction with this technique. The ionic charge, chosen as the equilibrium charge state for this collision system, was determined from the semiempirical tabulations of Ziegler (1980). The calculation without the model potential utilized a Coulomb potential with a single, constant screening parameter to represent this interaction. We found that when the model potential was used, the stopping power increased by 15% and was entirely attributable to the enhanced binary peak cross section. Thus, in a solid or biological target where a high degree of damage is due to fast binary electrons the modelling and understanding of secondary damage will be directly related to the enhanced cross sections predicted.

7. Conclusion

We have shown that the enhancement of the binary peak produced by partially stripped ion impact relative to that from bare ion impact is a phenomenon which should be observed for a very broad spectrum of ions, especially at forward emission angles. It has been shown how these enhancements behave as a function of impact energy and projectile ionic and nuclear charge. Further, the prevalence of oscillations in the differential elastic cross section for target electrons scattered by partially stripped projectile ions with very small q/Z ratios indicates that double or perhaps even multiple peak structures should be observable near the binary peak region of the ionized electron spectrum. Finally, it has been emphasized that the consequences of these observations should be quite important for the understanding of ion–dense-target collisions, where a large fraction of the damage may be caused by binary electron emission. Thus, scalings based on either multiplying the bare ion impact cross sections by either q^2 or Z^2 are shown to be inadequate to predict the behaviour of the binary peak for clothed ions.

Acknowledgments

The authors gratefully acknowledge the Office of Fusion Research, US Department of Energy for their support and C O Reinhold for his collaboration in writing the computer codes on which the present work was based.

References

Berg H, Dörner R, Kelbch C, Kelbch S, Ullrich J, Hagmann S, Richard P, Schmidt-Böcking H, Schlachter A S, Prior M, Crawford H J, Engelabe J M, Flores I, Loyd D H, Pedersen J and Olson R E 1988 *J. Phys. B: At. Mol. Opt. Phys.* **21** 3929

Bernstein R B 1966 Quantum effects in elastic molecular scattering *Molecular Beams* ed J Ross (New York: Interscience) p 75

Bonsen T F M and Vriens L 1970 *Physica* **47** 307

Brauner M, Briggs J S and Klar H 1989 *J. Phys. B: At. Mol. Opt. Phys.* **22** 2265

Chew G F 1950 *Phys. Rev.* **80** 196

Child M S 1974 *Molecular Collision Theory* (London: Academic)

Coleman J P 1969 *Case Studies in Atomic Collisions* vol 1, ed E W McDaniel and M R C McDowell (Amsterdam: North-Holland) p 99

Dressendorfer P V 1989 *Nucl. Instrum. Methods* B **40/41** 1291

Duncan M M and Menendez M G 1981 *Phys. Rev.* A **23** 1085

Faìnstein P D, Ponce W H and Rivarola R D 1988a *J. Phys. B: At. Mol. Opt. Phys.* **21** 287

—— 1988b *J. Phys. B: At. Mol. Opt. Phys.* **21** 2989

Ford K W and Wheeler J A 1959 *Ann. Phys., NY* **7** 259

Garcia J D, Gerjuoy E and Welker J E 1968 *Phys. Rev.* **165** 66

Garvey R H, Jackman C H and Green A E S 1975 *Phys. Rev.* A **12** 1144

Gerjuoy E 1966 *Phys. Rev.* **148** 54

Goldberger M L and Watson K M 1964 *Collision Theory* (New York: Wiley)

Gryzinski M 1959 *Phys. Rev.* **115** 374

—— 1965a *Phys. Rev.* **138** A305

—— 1965b *Phys. Rev.* **138** A327

—— 1965c *Phys. Rev.* **138** A336

Green A E S, Sellin D L and Zachor A S 1969 *Phys. Rev.* **184** 1

Jagutzki O, Hagmann S, Schmidt-Böcking H, Schultz D R, Dörner R, Koch R, Skutlartz A, Gonzalez A, Kelbch C and Richard P 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 2579

Johnson B R 1973 *J. Comput. Phys.* **13** 445

Joachain C J 1983 *Quantum Collision Theory* (Amsterdam: North-Holland)

Katz R 1988 *Quantitative Mathematical Models in Radiation Biology* ed J Kiefer (Berlin: Springer) p 57

Kelbch C, Hagmann S, Kelbch S, Mann R, Olson R E, Schmidt S and Schmidt-Böcking H 1989 *Phys. Lett.* **139A** 304

Kessler J 1985 *Polarized Electrons* (Berlin: Springer)

Kraft G 1987 *Nucl. Sci. Appl.* **3** 1

Lee D H, Richard P, Zouros T J M, Sanders J M, Shinpaugh J L and Hidmi H 1990 *Phys. Rev.* A **41** 4816

Lindhard J 1976 *Nucl. Instrum. Methods* **132** 1

McDowell M R C and Coleman J P 1970 *Introduction to the Theory of Ion-Atom Collisions* (Amsterdam: North-Holland)

Olson R E 1989 *Rad. Eff. Defects Solids* **110** 1

Olson R E, Gay T J, Berry H G, Hale E B and Irby V D 1987 *Phys. Rev. Lett.* **59** 36

Olson R E, Reinhold C O and Schultz D R 1990a Ionized electron spectra in energetic heavy ion-atom collisions *AIP Proc. of X-90, 15th Int. Conf. on X-ray and Inner Shell Processes* p 352

—— 1990b *J. Phys. B: At. Mol. Opt. Phys.* **23** L455

Quinteros T and Reading J F 1991 *Nucl. Instrum. Methods* B to be published

Price W E and Cross J R 1989 *Nucl. Instrum. Methods* B **40/41** 1306

Reinhold C O, Falcon C A and Miraglia J E 1987 *J. Phys. B: At. Mol. Phys.* **20** 3737

Reinhold C O and Olson R E 1989 *Phys. Rev.* A **39** 3861
Reinhold C O, Schultz D R and Olson R E 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** L591
—— 1991a *Nucl. Instrum. Methods* B **56/57** 271
Reinhold C O, Schultz D R, Olson R E, Kelbch C, Koch R and Schmidt-Böcking H 1991b *Phys. Rev. Lett.* **66** 1842
Reinhold C O, Schultz D R, Olson R E, Toburen L H and DuBois R D 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** L297
Richard P, Lee D H, Zouros T J M, Sanders J M and Shinpaugh J L 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** L213
Rodberg L S and Thaler R M 1967 *The Quantum Theory of Scattering* (New York: Academic)
Rudd M E and Jorgensen T 1963 *Phys. Rev.* **131** 666
Rudd M E, Sauter C A and Bailey C L 1966 *Phys. Rev.* **151** 20
Schultz D R, Reinhold C O and Olson R E 1991 *Nucl. Instrum. Methods* B to be published
Shingal R, Chen Z, Karim K R, Lin C D and Bhalla C P 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** L637
Stolterfoht N 1978 *Structure and Collisions of Ions and Atoms* (*Topics in Current Physics* **5**) ed I A Sellin (Berlin: Springer) p 155
Stolterfoht N, Schneider D, Burch D, Wieman H and Risley J S 1974 *Phys. Rev. Lett.* **33** 59
Stolterfoht N, Schneider D, Tanis J, Altervogt H, Salin A, Fainstein P D, Rivarola R, Grandin J P, Scheurer J N, Andriamonje S, Bertault D and Chemin J F 1987 *Europhys. Lett.* **4** 899
Taulbjerg K 1990 *J. Phys. B: At. Mol. Opt. Phys.* **23** L761
Toburen L H, Metting N F and Brady L A 1989 *Nucl. Instrum. Methods* B **40/41** 1275
Toburen L H, Stolterfoht N, Ziem P and Schneider D 1981 *Phys. Rev.* A **24** 1741
Toburen L H and Wilson W E 1979 *Phys. Rev.* A **19** 2214
Toburen L H, Wilson W E and Popowich R J 1980 *Radiat. Res.* **82** 27
Vriens L 1969 *Case Studies in Atomic Collisions* vol 1, ed E W McDaniel and M R C McDowell (Amsterdam: North-Holland) p 335
Wang J, Reinhold C O and Burgdörfer J 1991 *Bull. Am. Phys. Soc.* **36** 1295
Ziegler J F 1980 *Handbook of Stopping Cross-sections of Energetic Ions in All Elements* vol 5 (New York: Pergamon)