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EFFECTIVE CHARGE OF ENERGETIC HEAVY IONS IN GASES, SOLIDS AND PLASMAS

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Abstract

The effective stopping-power charge $q_{\text{eff}}$ for partially stripped ions is determined by a balance of the electron capture and loss cross sections within the stopping medium. The consequences for $q_{\text{eff}}$ of relative changes in these cross sections are considered for nearly fully stripped ions and for partially stripped ions.

Two physical factors leading to such changes are density effects in the stopping medium, and plasma temperature effects. This paper concentrates on the role of density effects. Experimental observations of a genuine gas-solid density effect are discussed, and a new rigorous model of this effect for nearly fully stripped ions is presented.

Résumé

La charge effective $q_{\text{eff}}$ d'ions partiellement épluchés est déterminée par l'équilibre entre la capture électronique et le stripping du milieu ralentisseur. Les conséquences des variations des sections efficaces correspondantes sur $q_{\text{eff}}$, sont étudiées pour des ions quasi-complètement épluchés, et d'autres, de charge arbitraire. Les deux paramètres significants sont les effets de densité dans la cible, et les effets dus à la température du plasma. Ici, on se limite à la densité. On discute les observations expérimentales en cible solide et gazeuse, respectivement. On présente un nouveau modèle des effets de densité sur des ions quasi-complètement strippés. On discute les $dE/dx$ correspondants en milieu dense, qui peuvent varier sur 20 %. Le taux de stripping d'un ion lourd de faible charge est beaucoup plus élevé dans un solide que dans un gaz.
Implications for dE/dx in dense media are discussed, and are shown to be significant at the 20% level. Furthermore the stripping rate for a heavy ion of low charge state entering a medium will be considerably higher in a solid than in gas.

1. Introduction

The stopping power of a medium for a point projectile of charge $Z_1 e$ may be expressed as

$$\frac{dE}{dx} = N Z_2 \frac{4 \pi Z_1^2 e^4}{m v^2} \cdot L(Z_1, Z_2, v) \quad (1)$$

where $v$ is the projectile velocity, $m$ the electron mass, and $N$ the density of atoms of atomic number $Z_2$. The quantity $L$ depends slightly on the density of the medium (solid target wavefunctions are different from those in gases), and depends strongly on whether the target is in atomic or plasma form. Furthermore in plasmas $L$ is strongly temperature dependent. These effects in the stopping process relating to $L$ have received considerable attention in recent years.

For partially stripped, high-energy heavy ions, the ion still behaves very nearly as a point-like charge as regards the stopping process. For these ions, it is therefore sufficient to replace $Z_1$ in the $dE/dx$ formula by an effective charge $q_{\text{eff}}$, which is simply given by the root mean square charge $q_{\text{r.m.s.}}$ of the ions averaged over the charge-state distribution within the target medium.

In dilute gas targets, one can measure $q_{\text{r.m.s.}}$ directly by observing the charge-state distribution after the ions emerge from the target. However in solids, charge-state measurements with many-electron ions are affected by post-target autoionisation, which leads to a spurious increase in the apparent value of $q_{\text{r.m.s.}}$. Only in very recent measurements with nearly fully stripped ions (hydrogen-like and fully stripped) has it been established that a distinct gas-solid density effect in $q_{\text{r.m.s.}}$ does indeed exist.
Since both density effects and plasma temperature effects in
\( q_{r.m.s.} \) arise through changes in "charge-changing cross sections", we
begin in Section 2 by looking at the projectile charge state
distribution in terms of these cross sections. Transformation
formulae are given, relating changes in the electron capture and
loss cross sections, to changes in \( q_{\text{eff}} \). In Section 3 we consider
the effect of target density on the charge-changing cross sections,
and make a quantitative estimate of the density effect in the electron
loss cross section for highly stripped ions. Finally in Section 4
these results are combined to estimate the expected changes in \( q_{\text{eff}} \)
resulting from density effects, and some brief remarks on plasma
temperature effects are presented.

2. Charge-changing cross sections and the effective charge

Visualise an ion of velocity \( v \) and atomic number \( Z_1 \), incident
on two targets A and B having the same atomic number \( Z_2 \). Targets
A and B may have different densities or temperatures, and the
charge-changing cross sections within these targets may therefore
be different. We consider the effect of such differences in cross
sections on the charge \( q_{r.m.s.} \), for two regions of projectile
velocity where straightforward approximations are possible.

(a) Nearly fully-stripped ions

For velocities in the region \( v \leq Z_1 v_0 \), projectile ions are nearly
fully-stripped of their electrons\(^6\). In this case we may assume that the
charge-state distribution is composed of two charge states: the fully
stripped ion (labelled 0) and the one-electron ion (labelled 1). The
root mean square charge is then given by

\[
q_{r.m.s.}^2 = Z_1^2 \phi_0 + (Z_1 - 1)^2 \phi_1 \\
= (2Z_1 - 1) \phi_0 + (Z_1 - 1)^2
\]

(2)

where \( \phi_i \) denotes a charge-state fraction.

Now let the ratios of the electron loss cross section \( \sigma_L \) and of
the electron capture cross section \( \sigma_c \) in targets A and B be given by

\[
R_k = \frac{\sigma_k^B}{\sigma_k^A}
\]

and

\[
R_c = \frac{\sigma_c^B}{\sigma_c^A}
\]

Then it can easily be shown that

\[
(\phi_0)_B = \left[ 1 + \frac{1 - \phi_0}{\phi_0} - \frac{R_c}{R_k} \right]^{-1}
\]

The combination of eqns. (2) and (5) shows how changes in the charge-changing cross sections influence the root mean square charge of the projectile.

(b) Partially-stripped ions

For velocities in the region \( v_0 \ll v < Z_1v_0 \), projectile ions in atomic targets possess many bound electrons. A reasonable approximation to the charge-state distribution in this case is given by

\[
\phi_i = (2\pi a^2)^{-\frac{1}{2}} \exp \left[ - (q - \bar{q})^2 / (2a^2) \right]
\]

where \( i \) denotes the number of electrons bound to the ion \( (q = Z_1 - i) \).

In order to estimate the shift in \( \bar{q} \) due to changes in the electron loss and capture cross sections, it is convenient to make two supplementary assumptions. Firstly, we assume that the single-electron loss and capture cross sections for all initial charge states \( i \) (written \( \sigma_L^i \) and \( \sigma_c^i \)), are still given by eqns. (3) and (4) irrespective of the value of \( i \). In other words the quantities \( R_k \) and \( R_c \) are assumed independent of the initial charge state. Secondly, we assume that the charge-state distribution is dominated by single electron loss and capture processes, rather than by double charge-exchange. This assumption is good for high-energy ions, where charge-exchange cross sections are reasonably small. It may then be shown that the shift in the mean charge state between targets B and
A is given by

\[ \Delta \bar{q} = \bar{q}_B - \bar{q}_A = S^2 \ln (R_B/R_C) \]  

(6)

For present purposes, it is convenient to use the value of $S$ given by Betz and Schmelzer \(^8\), namely

\[ S = 0.27 \, z_1^{\frac{1}{2}} \]  

(7)

We shall also neglect the small difference between $\bar{q}$ and $q_{r.m.s.}$, and hence feel free to apply eqn. (6) to $q_{r.m.s.}$.

3. **Effect of target density on charge-changing cross sections**

It is customary to describe the charge-exchange process in terms of "charge-changing cross sections", as discussed above, treating the ionic charge states as if they were well defined initial and final states. Bohr and Lindhard argued in an early paper \(^9\) that this procedure leads to cross sections which are dependent on target density. In their picture, a low-density target allowed projectile excited states (formed either by ground-state excitation or by electron capture) to decay radiatively to the ground state before further collisions occurred. Conversely in a dense target, they saw these excited states as being rapidly ionized. This ionisation could occur for many-electron ions in a dense gas target as a result of rapid autoionisation, and in even denser targets such as solids it would occur due to the high frequency of ionising collisions experienced by excited projectile states.

In 1970, Betz and Grodzins stressed the importance of post-foil autoionisation on observed charge-state distributions of ions emerging from solids. \(^5\) Although this process occurs only in many-electron ions, its effects on the observed charge-states are then so dramatic that density effects occurring within the target have tended to be neglected in recent years. Uncertainty therefore remains as to the magnitude of any density effects in the charge-changing cross sections.
Since the charge-changing process for many-electron ions is highly complex, a rigorous discussion of the density effect is restricted in this paper to the case of nearly fully-stripped ions. However the rather concrete results obtained in this way will provide a useful pointer towards the possible behaviour for partially stripped, energetic heavy ions. To derive the charge-changing cross sections in dilute and dense media in terms of fundamental cross sections for projectile excitation, ionisation and electron capture, we consider only the following projectile states. These are the fully-stripped ion (labelled 0) and a number of states of the one-electron ion (labelled \( i \), where \( i = 0 \) refers to the ground state and \( i \geq 1 \) refers to excited states. State fractions are represented by \( \phi_i \), and cross sections are represented for example by \( \sigma_{10} \), where the subscript 0 refers to the initial state (here the fully-stripped ion) and the superscript 10 refers to the final state (here the ground state of the one-electron ion).

The evolution of the state populations with depth \( x \) in the target is governed by the three equations

\[
\frac{d\phi_0}{dx} = - (\sigma_{10} + \sigma_{11}) \phi_0 + \sigma_{10} \phi_{10} + \sigma_{11} \phi_{11}
\]

\[
\frac{d\phi_{11}}{dx} = - (\sigma_{11} + \sigma_{01}) \phi_{11} + \sigma_{11} \phi_0 + \sigma_{01} \phi_{10}
\]

\[
\phi_0 + \phi_{10} + \phi_{11} = 1
\]

where we have assumed for the sake of formal simplicity that only one excited state, \( \phi_{11} \), need be considered. By comparison, the more familiar rate equations based on charge-changing cross sections are given by only two equations,

\[
\frac{d\phi_0}{dx} = - \sigma_c \phi_0 + \sigma_e \phi_1
\]
\[ \phi_0 + \phi_1 = 1 \] 

(12)

where the nomenclature is the same as in Section 2.

Since the excited state \( \phi_{11} \) is more rapidly ionised than the ground state \( \phi_{10} \), the population \( \phi_{11} \) may be expected to adjust rather promptly to changes in \( \phi_{10} \) and \( \phi_0 \). It is therefore reasonable to assume that, after a short distance into a target, \( \phi_{11} \) is in quasi-equilibrium with respect to \( \phi_{10} \) and \( \phi_0 \); and one can then make the approximation \( d\phi_{11}/dx = 0 \) in equation (9). It is for this reason that the phenomenological description given by eqns. (11) and (12) can produce an acceptable approximation to the charge-state equilibration process. It is now possible to derive \( \sigma_c \) and \( \sigma_L \) in terms of the more fundamental cross sections of equations (8) and (9). Setting \( d\phi_{11}/dx = 0 \) in equation (9) yields

\[
\phi_{11} = \frac{\phi_0^{11} \phi_0 + \phi_1^{11} \phi_1}{\phi_0 + \phi_0^{10} + \phi_1^{11}}
\] 

(13)

Combining equations (8) and (13) leads to the results

\[
\sigma_c = \sigma_0^{10} + (1 - \eta) \sigma_0^{11}
\] 

(14)

\[
\sigma_L = \sigma_0^{10} + \eta \sigma_0^{11}
\] 

(15)

\[
\eta = (\sigma_0^{11} - \sigma_0^{10})/(\sigma_0^{11} + \sigma_1^{11} + \sigma_0^{10})
\] 

(16)

These formulae include the effect of radiative decay of the \( 11 \) state to the \( 10 \) ground state, if we define \( \sigma_{11}^{10} \) to be an effective cross section

\[
\sigma_{11}^{10} = \sigma_{11}^d + \lambda_{11}/Nv
\] 

(17)

where \( \lambda_{11} \) is the radiative decay rate of state \( 11 \), \( N \) is the number
density of target atoms, \( v \) is the ion velocity and \( \sigma_{\text{11}}^d \) is the collisional de-excitation cross section from state 11 to the ground state. (Since \( \sigma_{\text{11}}^d \) is in fact too small to be significant for our purposes, it will be dropped in the remaining discussion). The relative importance for the charge-changing cross sections of excited-state ionisation and radiative de-excitation, depends on the value of \( N \), the target density. In the limiting case of a low-density target (\( N \to 0 \)), we have \( \sigma_{\text{11}}^\text{10} \to \infty \) and hence

\[
\eta + \eta_g = 0 \tag{16a}
\]

We shall call this the 'gas target' case although in reality it only applies to reasonably dilute gases. In the limiting case \( N \to \infty \) appropriate to a solid) \( \sigma_{\text{11}}^\text{10} \to 0 \) and hence

\[
\eta + \eta_s = (\sigma_{\text{11}}^0 - \sigma_{\text{10}}^0)/(\sigma_{\text{11}}^0 + \sigma_{\text{10}}^0) \tag{16b}
\]

Thus equations (14) - (16) are applicable to both gas and solid targets, with \( \eta_g = 0 \) and \( \eta_s \) as given by equation (16b). Substitution of \( \eta = \eta_g, \eta_s \) in equations (14) and (15) yields the difference between the solid and gas target charge-changing cross sections, \( \Delta \sigma = (\sigma)^\text{solid} - (\sigma)^\text{gas} \), in the very simple form

\[
\Delta \sigma_c = -\eta_s \sigma_{\text{11}}^0 \tag{18}
\]

\[
\Delta \sigma_x = \eta_s \sigma_{\text{11}}^\text{10} \tag{19}
\]

It may be shown that there is good justification for incorporating many excited states into the present description, simply by adding their contributions to \( \Delta \sigma_c \) and \( \Delta \sigma_x \) linearly. For \( n \) excited states we have, dropping the subscript \( s \) from \( \eta_s \),

\[
\Delta \sigma_c = -\sum_{i} \eta_i \sigma_{\text{i1}}^0 \tag{21}
\]
The corresponding gas-target cross sections simply generalise to:

$$\Delta \sigma \xi = \sum \eta_i \sigma_{1i}^0$$

$$\eta_i = (\sigma_{1i}^0 - \sigma_{10}^0) / (\sigma_{1i}^0 + \sigma_{10}^0)$$

The results presented in eqns. (21 - 25) give definite meaning to the charge-changing cross sections in both gases and solids. The density effect, eqns. (21 - 23) clearly reflects the qualitative arguments of Bohr and Lindhard. The $\sigma_{0i}^0$ term in eqn. (21) corresponds to the physical fact that capture to an excited state in a solid is followed rapidly by collisional ionisation, a channel which does not exist in a dilute gas. The $\sigma_{10}^i$ term in eqn. (22) corresponds to the additional channel in the solid-target loss cross section due to excitation followed by rapid ionisation. The numerical quantity $\eta_i$ ($\eta_i < 1$) accounts physically for the time delay between the formation of the excited state $i$ and its subsequent ionisation. $\eta_i$ is unity in the limiting case of $\sigma_{1i}^0 \rightarrow \infty$, as has been described previously.

Some useful general observations can be made about excitation and ionisation cross sections, from which a quantitative estimate of the density effect ratio in the loss cross section $\sigma \xi$ can be made. The theory of electron loss from fast one-electron ions indicates that the ionisation cross sections $\sigma_{10}^0$, $\sigma_{1i}^0$ are inversely proportional to the binding energy of the initial state. Evidence from resonant coherent excitation of channelled ions has indicated that a finite number of ionic bound states can exist within a solid, and that the binding energies for the low-lying excited states are only moderately perturbed.
from their vacuum equivalents. Further evidence for this view comes from the recent observations of non-equilibrium effects in the proton neutral fraction emerging from solids bombarded with MeV H beams, which suggest that even for protons a strongly correlated proton-electron configuration can exist in a solid. Consequently if one identifies the state label \( i \) with \( (n-1) \), where \( n \) is the principal quantum number, one has

\[
\frac{\sigma_{11}^0}{\sigma_{10}^0} \sim n^2 \quad (26)
\]

In order to estimate density effects, additional information is needed on the fraction of the ground-state destruction cross section which leads to excitation of the one-electron ion, as opposed to ionisation. Predictions for this ionic excitation fraction for collisions in which the target atom undergoes excitation simultaneously, have been made by Gillespie using the Born approximation.\(^{14}\) The excitation fraction

\[
f_{ex} = \frac{\sum_{i} \sigma_{1i}^0}{\sigma_{10}^0 + \sum_{i} \sigma_{1i}^0} \quad (27)
\]

varies from about 0.2 for H ions to nearly 0.6 for ions with \( Z = 30 \), and is only a very weak function of target atomic number. For illustrative purposes, therefore, we take the values of \( f_{ex} \) from ref. 14 for the case of an N target atom, and use equations (26) and (27) to estimate limits to the density-effect ratio \( D_k = (\sigma_k)_{\text{solid}} / (\sigma_k)_{\text{gas}} \).

The results are shown in Fig. 1 as a function of ion atomic number \( Z_1 \). The upper solid curve corresponds to the assumption that all excitation leads to highly excited states \( (n \rightarrow \infty) \), while the lower solid curve corresponds to the assumption that all excitation leads to the \( n = 2 \) state. Since the true situation lies somewhere between these two extremes, we arbitrarily choose an "adopted value" curve for Fig. 1, the dashed line, by drawing a straight line through the average of the extreme curves at \( Z_1 = 3 \) and \( Z_1 = 30 \).
Fig. 1 The density effect in the loss cross section for one-electron ions, as a function of ion atomic number $Z_1$. The upper and lower solid curves represent extreme theoretical estimates as described in the text of Section 3. The dashed line represents an "adopted value" curve as described in the text. The experimental datum comes from ref. 15, concerning density effects for $3 \text{ MeV/u}$ C ions in gaseous and solid carbon targets.

Figure 1 also shows experimental data obtained using $3 \text{ MeV/u}$ C ions incident on gaseous and solid C targets. (The gas target results were obtained by extrapolating data obtained with a number of hydrocarbon gases of different stoichiometry). The theoretical predictions are seen to be in excellent agreement with this experimental result.
As regards the density effect in the electron capture cross section, the complexity introduced by velocity matching rules out the prospect of a straightforward general result for the density-effect ratio $D_c$. Suffice it to say that since $D_c \leq 1$ (equations (21), (24)), this effect can only increase the density-effect in the r.m.s. charge (equations (5), (6)) already arising from the enhanced loss cross section.

4. Implications for the effective charge

(a) Density effects

For nearly fully-stripped ions, a density effect in the charge-changing cross sections as exemplified by Fig. 1 for the loss cross section, will have only a modest effect on $q_{\text{r.m.s.}}$. The largest effect for nearly fully-stripped ions occurs for light ions, since the charge difference between the fully-stripped ion and the one-electron ion is then an appreciable fraction of $q_{\text{r.m.s.}}$. For example, using $R_\infty = D_\infty$ as given by Fig. 1, and making the conservative assumption $R_c = D_c = 1$, equations (2) and (5) yield the following predictions for the density effect in the r.m.s. charge, $D_q = (q_{\text{r.m.s.}})_{\text{solid}}/(q_{\text{r.m.s.}})_{\text{gas}}$: When the charge fractions $\phi_0$ and $\phi_1$ are equal, one obtains for C ions, $D_q = 1.02$; and for Li ions, $D_q = 1.04$. For H and He ions, the density effect is unlikely to operate as described by our model, since there are probably no bound excited states in a solid. For these ions, any density effect is more likely to result from the modification of the projectile ground-state binding energy as a result of screening by target electrons.

For partially stripped, many-electron ions at MeV/u energies, equations (6) and (7) are valid. Combining these equations, one obtains (again assuming $D_c = 1$),

$$\frac{\Delta q}{Z_1} = 0.073 \ln D_q$$  \hspace{1cm} (28)
Application of the density effect \( D \) presented in Fig. 1 to such ions is not strictly valid. However in the absence of more reliable predictions it forms a worthwhile basis for estimating high energy heavy-ion effective charges, especially since very little experimental \( \frac{dE}{dx} \) data is as yet available for these ions.

As an illustration, we apply this estimate to the case of 3.6 and 7.9 MeV/u \( U \) ions, the only example to date of a high-energy heavy ion for which both gas and solid-target stopping powers have been measured\(^{18}\). The prediction is \( \Delta \bar{q} = 4.6 \) at 3.6 MeV/u and \( \Delta \bar{q} = 4.9 \) at 7.9 MeV/u for \( U \) ions, in excellent agreement with the experimental data. These values correspond to differences of about 20\% between the stopping powers in solid and gaseous targets.

So far we have considered only the density effect on the ion effective charge after the ion has reached charge-state equilibrium. However, as Fig. 1 shows, the stripping rate for an ion incident in a low charge state may be expected to be substantially higher in a dense medium than in a dilute gas. For example, on the basis of measured charge-changing cross sections for 3 MeV/u \( C \) ions in gaseous and solid \( C \) targets, one expects equilibrium to be approached \( \sim 1.6 \) times faster in the solid targets. Considerations of this kind may be of importance in treating the ablation behaviour of ion-beam heated ICF targets.

(b) Plasma temperature effects

Detailed discussion of plasma temperature effects on the effective charge has been given recently by Nardi and Zinnamon\(^{19}\). However for completeness we describe briefly how such effects come about from the simplified viewpoint given in Section 2. Equation (6) predicts for a partially-stripped ion the shift in the effective charge arising from changes in the underlying charge-changing cross sections. \( R_L \) and \( R_C \) now represent the ratios of the electron loss (\( \lambda \)) and capture (\( c \)) cross sections in the plasma and the cold targets. It is clear that, unless some dramatic effect occurs in either \( R_L \) or \( R_C \),
the logarithm term will ensure that the temperature effect on $\Delta q$ will be modest. The important physics behind the temperature effect is that, in a hot plasma, the electron capture cross section may indeed be dramatically reduced because the target electrons relevant to electron capture may no longer be bound. Thus instead of direct capture of bound electrons as in cold matter, capture may only proceed by REC or by dielectronic recombination, processes whose cross sections are orders of magnitude smaller. As a result, plasma temperature effects in the effective charge can make a substantial contribution towards enhancing the stopping power in hot plasmas.

References

4. In processes where small impact parameters are of dominant importance, such as target inner-shell ionisation of heavy targets, some consideration of the form factor of the ion has to be included. This, however, is not the case for stopping powers of MeV/u ions. See for example W.Brandt and M.Kitagawa, Phys.Rev. B 25, 5631 (1982).