Electronic screening in heavy-ion—atom collisions

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A model is developed to describe the effects of screening by projectile electrons in heavy-ion—atom collisions. The effective nuclear charge of the projectile is estimated as a function of the interaction distance based on the spatial distribution of bound electrons derived from their electronic wave functions. Correlation of the effective interaction distance with collisional energy transfer through the Massey criterion enables comparison of model predictions of effective projectile charge with results obtained from differential-ionization-cross-section measurements. The model is found to provide a reliable estimate of screening for measurements involving fast helium and oxygen ions.

In heavy-ion collisions the interaction probabilities are strongly influenced by the electronic structure of the incident ion. Electrons bound to the incident ion screen the nuclear charge thus weakening the interaction potential. Analysis of ionization cross sections, differential in the energy of ejected electrons, has shown that the degree of screening is a strong function of the collisional energy transfer.[1-4] For interactions involving small energy transfer the bound electrons provide effective screening of the nuclear charge of the projectile, whereas for large energy transfer the screening is negligible. In this paper we make use of the correlation between energy transfer and the adiabatic interaction radius provided by the Massey criterion to obtain a model for the screening of the nuclear charge by electrons bound to the projectile. This result coupled with the Z^2 dependence of ionization cross sections predicted by the plane-wave Born approximation or binary-encounter theory provides a simple prescription for relating the cross section for ionization by structured ions to the cross section for ionization by bare ions. If valid, such a prescription would be particularly important in research areas such as radiological physics, radiation damage to materials, and plasma heating and confinement, where energy loss by ionization is the dominant process for heavy ions.

An interpretation of the effective nuclear charge of a heavy-ion projectile as a function of an effective interaction distance was first discussed by Stolterfoht[1] in his analysis of differential-ionization cross sections for fast oxygen ions. In that work correlation of energy transfer ΔE, where ΔE is taken as the kinetic energy of the ionization electron plus its initial binding energy, with a characteristic interaction distance, the adiabatic interaction radius R_{ad}, was established by means of the Massey criterion such that

$$R_{\mathrm{ad}} = v/\Delta E \ , \tag{1}$$

where v is the incident ion velocity. All quantities in Eq. (1) are given in atomic units. This application of the Massey criterion clearly illustrates that small energy transfers correlate with interactions at large internuclear distances where bound electrons provide effective screening, whereas large energy transfers occur when the projectile deeply penetrates the target atom and screening by the projectile electrons is unimportant. In fast heavy-ion collisions, the effective interaction distance may vary by orders of magnitude and involve distances where the effective nuclear charge is rapidly changing.

Although there is a considerable amount of data available on differential-ionization cross sections for heavy-ion—atom collisions which provide detailed information on the interaction processes,[1-4] little theoretical work has been advanced to provide a quantitative description of the effects of screening. Methods for incorporating screening into calculations using the Born approximation have been discussed by Briggs and Taulbjerg[5] and applied by Losonski[6] to inner-shell ionization. Recently, results of Born calculations including screening have also been presented by Manson and

Toburen[7] for He^+-He collisions and by Kaminsky *et al.*[8] for ionization by neutral hydrogen. These calculations indicate that the Born approximation may provide reliable cross sections, at least for simple collision systems. In the Born approximation the effective charge of the projectile is a function of the momentum transfer and can be either reduced (screened) or enhanced (antiscreening) by the bound electrons of the collision partners.[5] For a given energy loss, a mean projectile charge can be defined by an integral over the range of momentum transfer consistent with conservation of energy and momentum. This method for calculating the screening as a function of energy loss would, in general, require wave functions for both the target and the projectile. However, if the minimum momentum transfer is considered to be approximately independent of the final state of the projectile, the differential cross sections within the Born approximation separate into a product of one term which depends only on the projectile wave functions and the second which depends only on the target.[5,9]

The concept of separability of target and projectile properties derived from the first-order Born approximation where the minimum momentum transfer is assumed independent of the final state of the projectile, together with the concept of static screening provides a theoretical basis for the present work. In this work we develop a simple analytic model to describe the static screening of the projectile as a function of the collisional energy transfer based on the charge distribution of projectile electrons. The utility of this model, where valid, is that cross sections for ions with bound electrons can be derived from data for bare ions without extensive theoretical computation as would be involved with a complete theoretical treatment, e.g., the Born approximation. Our intent is to illustrate a simple means by which one can approximate the screening by projectile electrons which involve only the wave functions of the projectile and to test the results of this model using published data on differential-ionization cross sections for helium and oxygen ions.

In the present model the effective nuclear charge of the incident ion is defined as

$$Z_{\mathrm{eff}}(R)=Z-S(R)\ , \tag{2}$$

where $S(R)$ is the screening of the nuclear charge Z when viewed at a distance R from the nucleus. The screening function $S(R)$ is derived from the spatial distribution of projectile electrons such that

$$S(R)=\sum_i N_i \int_0^R |\psi_i(r)|^2 r^2 dr\ , \tag{3}$$

where $\psi_i(r)$ is the normalized radial wave function for the ith bound electron and N_i is the number of electrons in the ith subshell. In Eq. (3) we treat the electrons classically and determine their contribution to screening by integration of the static charge distributions. To this point, R is not specified; in order to extend this concept to a simple model of the effective projectile charge relevant to energy-loss cross sections we will set R equal to the adiabatic radius R_{ad} given by the Massey criterion, Eq. (1). This defines a unique effective interaction distance for each value of energy loss, although the actual energy loss may have contributions from a range of interaction distances. This approximation enables one to obtain an effective projectile charge for structured ions in a relatively simple way which can be used to scale energy-loss cross sections from bare-ion data.

The screening function $S(R)$ may be evaluated by different methods; in this work we have performed the integration analytically using hydrogenic wave functions. In several cases these results were compared with numerical solutions using the Hartree-Fock program of Froese-Fisher.[10] For hydrogenic wave functions and using atomic units throughout, the analytic solution to the screening function for an electron in the 1s, 2s, or 2p atomic subshell is given by

$$S(R)_{1s}=1-e^{-2\hat{R}}(1+2\hat{R}+2\hat{R}^2)\ , \tag{4a}$$

$$S(R)_{2s}=1-e^{-2\hat{R}}(1+2\hat{R}+2\hat{R}^2+2\hat{R}^4)\ , \tag{4b}$$

$$S(R)_{2p}=1-e^{-2\hat{R}}(1+2\hat{R}+2\hat{R}^2+\tfrac{4}{3}\hat{R}^3+\tfrac{2}{3}\hat{R}^4)\ , \tag{4c}$$

where $\hat{R}=R\ Q_{\mathrm{eff}}/n$ is a scaled length equal to the distance R multiplied by the effective nuclear charge Q_{eff}. Here Q_{eff} is the effective nuclear charge experienced by an electron bound in the nth subshell of the ion under consideration. The utility of this definition of R is that the expressions of Eq. (4) can readily be scaled to various atomic systems by using estimated values of the appropriate effective nuclear charge.[11] One can also extend the set of expressions shown in Eq. (4) to larger principal quantum numbers. However, it should be noted that the use of hydrogenic wave functions becomes less accurate as the principal quantum number increases.

The reliability of the screened projectile charge derived from this simple screening model can be tested by comparison with recent measurements of differential-ionization cross sections for helium and oxygen ions. In order to derive the effective nuclear charge of the incident ion from the measured cross sections we asssume the cross sections are proportional to the square of the projectile charge. This Z^2 dependence is predicted by first-order collision theory[12,13] and has been confirmed by measured differential cross sections for bare charged particles.[3,4] With this and the assumption that target properties cancel in the ratio,[5,9] the effective projectile charge for a screened projectile can be estimated as a function of energy transfer from the measured differential cross sections as

$$Z_{\text{eff}}(\Delta E)=Z\left[\frac{d\sigma(q)}{dE}\bigg/\frac{d\sigma(Z)}{dE}\right]^{1/2}, \qquad (5)$$

where $d\sigma(q)/dE$ is the measured differential cross section for an incident ion with charge q and $d\sigma(Z)/dE$ is the measured differential cross section for the bare ion. The energy-loss cross sections are derived from secondary electron emission cross sections with the energy loss ΔE set equal to the valence binding energy plus the kinetic energy of the ejected electron. This estimate of ΔE is also used, via Eq. (1), to correlate interactions involving specific energy loss with an adiabatic interaction distance. This enables direct comparison of model calculations of an effective projectile charge with experimentally determined values.

A comparison of the effective nuclear charge obtained from the model calculation with that derived from experimental results for helium ion impact is shown in Fig. 1 as a function of the adiabatic interaction radius. The solid line is the result of our model calculation for He^+ and the data points are from measurements for several energies of He^+ and He^{2+} impact ionization on argon.[3] The dotted curve represents the average projectile charge that was presented in Ref. 4 for ionization of water vapor by 0.8- to 2-MeV helium ions. Since the dotted curve represents an average for a range of ion energies, horizontal error bars are shown to indicate the corresponding range in adiabatic radius derived from the Massey criterion. The rapid decrease in the effective nuclear charge of the He^+ ion obtained from the present screening model when the adiabatic radius exceeds approximately 0.2 a.u. is clearly confirmed by the measurements for ionization of water vapor and by the low-energy measurements for ionization of argon. This shows that the basic features of the screening are reproduced by the present model.

Discrepancies between the model calculations and the cross-section ratios for ionization of argon in the region from 0.4 to 1.5 a.u. are observed in Fig. 1 to increase with increasing ion energy. These discrepancies are attributed to contributions of electron loss from the projectile which are included in the experimental data but not included by the model. The model calculations apply only to ionization of the target by a structured ion whereas the experiment does not distinguish between target and projectile ionization. Thus, the experimental ratio from which we obtain the measured effective charge will be enhanced in the portion of the spectrum where electrons from projectile ionization are observed. The arrows labeled A, B, and C in Fig. 1 illustrate the approximate positions where the maximum contribution by electron loss is expected for ion energies of 1.2, 0.8, and 0.3 MeV, respectively. For the dotted curve derived from measured ionization cross sections for water vapor the average effective nuclear charge was obtained after an approximate subtraction of the contribution of projectile ionization.[4] It should be noted that for the lowest ion energies studied, little, if any, projectile ionization is expected.[3,4] The good quantitative agreement with the low-energy ion data and with the water-vapor data where contributions from projectile ionization have been estimated and removed provide confidence in the reliability of the model calculation.

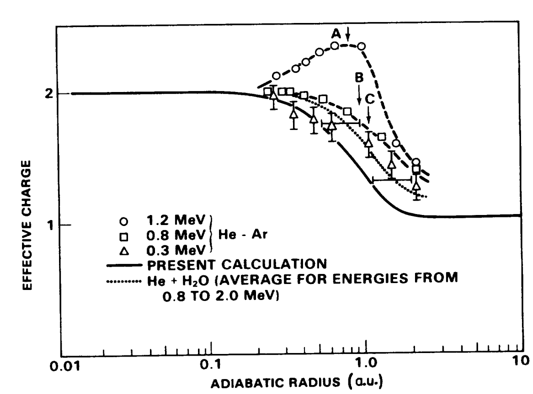

FIG. 1. The effective charge of an incident He^+ ion is shown as a function of the adiabatic interaction radius. The solid curve is from the present screening model. The data points are for ionization of argon by He^+ and He^{2+} impact (Ref. 3) and the dotted line represents the average effective charge presented in Ref. 4 for ionization of water vapor. The arrows labeled A, B, and C indicate regions where the maximum contribution of electron loss would be expected in the experimental data for 1.2-, 0.8-, and 0.3-MeV ions, respectively.

As a further example of the screening model we have calculated the effective nuclear charge of O^{n+} ($n=4-7$) ions as a function of the adiabatic interaction distance for ionizing collisions involving 30-MeV ions. For these calculations Eq. (3) was evaluated using both the hydrogenic approximation of Eq. (4), with $Q_{\rm eff}$ derived from Slater's rules,[11] and the Hartree-Fock wave functions of Froese-Fisher.[10] The results of these calculations differ, at most, by a few percent. The results of the model calculations using Hartree-Fock wave functions are shown in Fig. 2 together with the analysis of 30-MeV O^{n+} ($n=4-8$) data for ionization of molecular oxygen.[1,2] In general, the agreement between the screening model, represented by the solid line, and the experimental results are good.

The model calculations clearly illustrate the differences in the spatial distributions of the 1*s* and 2*s* electrons of the oxygen ion. These are observed as inflections in the curves at approximately 0.3 and 2 a.u. for the 1*s* and 2*s* electronic shells, respectively. This shell effect is, however, not reflected in the experimental data due to influence of electron loss from the projectile. The actual shape of the experimental curves for charge states 4, 5, and 6 could not be determined directly for adiabatic radii from 0.2 to 0.8 a.u. because of the large contribution of electron loss in the measured cross sections; this region is indicated by the dashed curves in Fig. 2. One may also expect a small contribution of electron loss in the O^{7+} cross sections which could explain the shift in the minimum value of the measured effective charge to somewhat larger interaction distances than given by the screening model.

In contrast to the helium data of Fig. 1, the experimental values for oxygen impact tend to fall somewhat below the model predictions. These differences for the oxygen data are, however, of the order of 15% which is within the relative uncertainties of the experimental data. Furthermore, the experimental results for oxygen ion impact are for double-differential cross sections rather than single-differential cross sections as were illustrated for helium ions in Fig. 1. The present screening model incorporates no information regarding angular distributions of the electrons ejected in the energy-transfer process. It has been observed, however, in the study of double-differential-ionization cross sections, that there is some evidence of an angular dependence of the ratios of cross sections for He^{+} impact to He^{2+} impact.[3,4] Such an angular

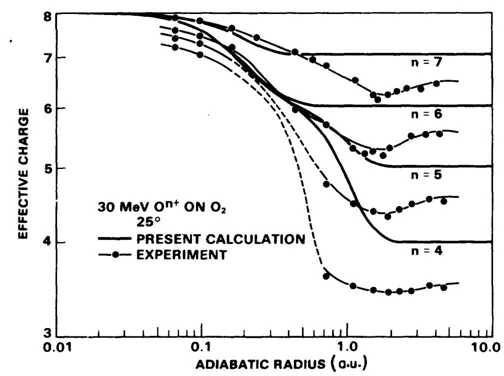

FIG. 2. The effective nuclear charge for 30-MeV oxygen ions is shown as a function of the adiabatic interaction radius. The heavy solid curves represent model predictions and the data points are from the data of Ref. 2. The dashed lines represent an interpolation of the experimental data in the region dominated by electronic loss from the projectile.

dependence in the oxygen data may be expected to influence the absolute values of the ratios shown in Fig. 2. Unfortunately sufficient experimental data does not exist to allow integration of the double-differential cross sections so that a more definitive comparison can be made.

Comparison of the present screening model with results derived from differential-ionization cross sections are, for the most part, within the uncertainties to the experimental data. The most significant differences, however, may indicate a breakdown of Z^2 scaling or inappropriate use of the Massey criterion for estimating the characteristic distance at which the interaction occurs. The latter has not been quantitatively tested over such an extended range of collision parameters as is represented in the present work. In addition, the present technique averages over the interaction path of the projectile and the dynamics of the interaction are disregarded. Further experimental work will be necessary to provide the data to test more conclusively the range of applicabilty of the screening model and to determine the effects of electronic structure in more complex systems.

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