Multiple ionization of atoms and molecules in collisions with fast ions: Ion-atom collisions

N. M. Kabachnik,[1,*] V. N. Kondratyev,[1,2,†] Z. Roller-Lutz,[1] and H. O. Lutz[1]
[1]*Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld, Germany*
[2]*Advanced Science Research Center, Japan Atomic Energy Research Institute, Tokai, Naka, Ibaraki 319-11, Japan*
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A theoretical description of multiple ionization of atoms and molecules produced by an energetic ion impact is developed. It is based on the statistical energy-deposition model of Russek and Meli [Physica (Amsterdam) **46**, 222 (1970)]. In this model the probability for the formation of a collision-induced final state with n electrons in the continuum is obtained, assuming that its value is proportional to the volume of phase space available at that ionization state for a certain value of statistically distributed deposited energy. The model is extended in two respects. First, the deposited energy for each trajectory is considered as a fluctuating quantity with a certain distribution and the ionization probability is calculated as a weighted average over the distribution. Second, the mean value and straggling of the deposited energy are calculated within the Lindhard-Scharff local plasma approximation [Mat. Fys. Medd. K. Dan. Vidensk. Selsk. **27**, No. 15 (1953)]. Sample calculations for collisions of protons and F^{4+} ions with neon atoms at an energy of 1 Mev/amu are presented and compared with calculations within the independent-electron approximation and with experimental data. [S1050-2947(97)01310-3]

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I. INTRODUCTION

Multiple ionization of atoms and molecules by fast heavy ions attracts an ever increasing attention of both experimentalists and theoreticians due to its fundamental importance in many areas of science and technology. Moreover, it is an interesting subject in atomic physics from the point of view of understanding the basic processes of many-particle reactions (see, e.g., a review by Cocke and Olson [1]). A theoretical description of the ion-induced multiple ionization is complicated mainly due to the variety of mechanisms that may contribute to it as well as its multielectron nature, strongly related to electron-electron correlations. In addition to the direct Coulomb knockout of several electrons, processes such as shakeoff, fast Auger cascades after inner-shell ionization, transfer ionization, and excitation and multiple excitations followed by autoionization can contribute.

There are two basic approaches that are widely used for interpretation of the experimental results on multiple ionization. One is the independent-particle model (IPM) [2,3] and its extensions [4,5]. In this approach it is assumed that the ejection of a particular electron proceeds independently of the state of other electrons. The multiple-ionization probabilities for a given impact parameter are then given by a binomial (or multinomial) distribution based on single-electron-ionization probabilities. The latter are usually calculated within the first-order semiclassical approximation (SCA) (see, e.g., [6]). An attractive feature of this approach is its computational simplicity. However, it was recognized that the IPM suffers from some serious defects (see the discussion in [1]). For example, in this model it is ignored that the ionization potential changes considerably with the charge state, which leads to wrong probabilities for high stages of ionization. In addition, attempts to apply the IPM to molecules [7,8] involve additional rather crude approximations that practically ignore the molecular structure.

Another popular approach is the classical-trajectory Monte Carlo (CTMC) method in combination with the IPM [9] and its extension, the so-called n-body CTMC method [10]. In this method a Monte Carlo simulation of ion-atom collision is made by calculating the classical trajectories of the interacting projectile and target electrons, with the initial momentum distribution of the latter being calculated quantum mechanically. This method is flexible enough to include the electron-capture [11] and electron-loss [12] processes as well as autoionization. It provides a good description of multiple ionization; however, it is very time consuming, even with modern computers, since several thousand individual collision trajectories must be followed to obtain good statistics on the cross sections. This limits its application to more complicated targets such as molecules, especially multiatomic ones.

At an early stage of investigations the multiple ionization of atoms was also described in terms of a statistical energy-deposition (SED) model [13–16]. The model was originally suggested and developed by Russek and collaborators [13,14] for a description of the multiple ionization in slow ion-atom collisions in the domain of the quasimolecular Fano-Lichten approach [17]. Its most advanced version is described in detail by Russek and Meli [15]. The model is based on the assumption that the probability for the formation of a collision-induced final state with n electrons in the continuum is obtained assuming that its value is proportional to the volume of phase space available at that ionization state. The probability depends on the energy transferred by the projectile (deposited energy), which is assumed to be statistically distributed among all electrons of the system. The SED model was extended by Cocke [16] to the region of

*On leave from Institute of Nuclear Physics, Moscow State University, Moscow 119899, Russian Federation.
†On leave from Institute for Nuclear Research, 47, Pr. Nauki, Kiev 252028, Ukraine.

fast ion-atom collisions. Cocke also suggested to consider the energy deposition as being roughly due to the fast passage of a point charge through a cloud of target electrons. The latter was considered as a gas of free classical electrons. The calculations by Cocke within the SED model gave a reasonable estimate of the experimental cross sections for multiple ionization in 34-MeV Cl^{q+}-Ne collisions. However, the model overestimated the cross sections for small stages of ionization, which was attributed to the roughness of the calculation of the energy deposition.

In this paper we develop a modification of the SED model for a quantitative description of multiple ionization of atoms in ion-atom collisions in the energy range from several tens of keV to several MeV per atomic mass unit (amu). The Russek-Meli-Cocke model is extended in two respects. First, the deposited energy for each trajectory is considered as a fluctuating quantity with a certain distribution and the ionization probability is calculated as a weighted average over the distribution [14]. Second, the mean value and straggling of the deposited energy are calculated within the Lindhard-Scharff local- (electron) density approximation [18], which is known to give a good description of the ion energy loss in the considered energy range.

The main goal of the work is to develop a model that can be easily extended to a description of ion collisions with more complex multielectron systems such as molecules and clusters. However, at first we consider ion-atom collisions where experiments as well as other methods for calculation of multiple ionization cross sections exist with which we can compare our results. A full description of the model is given in the next section. Some examples of the application of the model in ion-atom collisions are discussed in Sec. III. We give conclusions in Sec. IV. We plan to describe an extension of the SED model to the case of ion-molecule collisions in a future work [19]. Atomic units are used throughout unless otherwise indicated.

II. EXTENDED STATISTICAL ENERGY DEPOSITION MODEL

We consider a collision of an ion with initial energy in the range 50 keV/amu to 5 MeV/amu with a multielectron target atom. We assume that the ion can be considered as a point charge Z_1 moving along the classical trajectory with a constant velocity v and impact parameter **b**. This is a common and well-justified approximation in the considered energy region. Moreover, we assume that the trajectory is a straight line; this is not a principal limitation since the deflection of the projectile can be easily incorporated into the model. When the ion collides with the target atom some of the translational energy of the ion is deposited in the electronic degrees of freedom. This energy is known to be much larger than the kinetic energy of the recoil, which we ignore in the following. The energy transfer causes excitation and ionization of target electrons with appreciable probabilities. The typical deposited energy considerably exceeds the ionization threshold. Therefore, numerous ionization channels are opened and a detailed quantum-mechanical treatment of the ionization problem is practically impossible. In this case the statistical approach appears to be attractive.

A. Russek-Meli-Cocke energy-deposition model

The statistical energy-deposition model [15] implies that the multiple-ionization process is viewed to proceed in two stages. In the first one, part of the kinetic energy of the projectile is transferred to electronic excitations of the target atom. Then, in the second stage, after the partners depart from one another, the deposited energy is distributed among all target electrons and the system subsequently autoionizes to reach its final ionization state. Here it is assumed that the electrons are removed slowly in comparison to the collision time.

The energy transferred in the collision (or rather the distribution of transferred energies) is considered as a reasonably well-defined function of the collision parameters and will be treated in Sec. II B. Given that the deposited energy is known, the probability for each final ionization level can be calculated as suggested by Russek and Meli [15]. It is proportional to the volume of phase space available in that ionization state and it is directly related to the deposited energy and the ionization potentials of the various levels.

As it was shown in [15], the probability of n-fold ionization for a certain deposited energy E_T can be expressed as

$$P_n^{(N)}(E_T)=\frac{\binom{N}{n} g^n S_n(E_k/\mathcal{E}_1)}{\sum_{i=1}^{N}\binom{N}{i} g^i S_i(E_k/\mathcal{E}_1)}. \tag{1}$$

Here N is the number of target electrons, $\binom{N}{n}$ is the binomial coefficient, and E_k is the kinetic energy available to the electrons if the residual ion is left in the nth ionization state. The relation between the energy deposited within the atom and the kinetic energy E_k carried off by the ionized electrons is given by

$$E_k=E_T-\sum_{i=1}^{n}\mathcal{E}_i-E_R(n), \tag{2}$$

where $\mathcal{E}_i$ is the ith ionization energy and $E_R(n)$ is the residual excitation of the remaining ion. The dimensionless parameter g is proportional to the mean-square matrix element of a single ionization (including autoionization, Auger processes, etc.) and it is supposed that for a multiple ionization the mean-square matrix element behaves according to a power law.

For the factor $S_n(E_k/\mathcal{E}_i)$ characterizing the density of the final states a simple expression was obtained [15]:

$$S_n(E_k)=2^{\{(n-1)/2\}}\pi^{\{n/2\}}E_k^{(3n-2)/2}/(3n-2)!!, \tag{3}$$

where $\{a\}$ means the integer part of a. All possible ways to reach the final state with n electrons in the continuum are considered as being equivalent. For example, fast Auger processes following an inner-shell ionization are also included in the consideration.

We note here that the SED model is semiphenomenological because the mean-square matrix element g is considered as a parameter. Russek and Meli argued [15] that it should be close to unity for slow ion-atom collisions. Cocke also used this value in his calculations [16]. However, it was shown

[15] that in fast processes the parameter g can be much smaller, of the order of 0.01. We treated g as a free parameter that should be chosen from a comparison with experiment. From our calculations it follows that for fast ion-atom collisions the value of g is much less than unity (see below) and varies slowly with the projectile charge and energy. This can be understood because the average matrix element of autoionization is to depend on the excitation energy of the system.

B. Calculation of energy deposition within the local-density approximation

In a collision of a fast structureless charged particle with one of the target atoms the deposited energy is equal to the electronic energy loss of the particle (with negative sign). Being a fluctuating quantity the energy deposition (or energy loss) is characterized by the mean value and energy straggling, i.e., the average-square fluctuation. In order to calculate the average energy loss and the energy straggling we use the well-known model suggested by Lindhard and Scharff [18], the so-called local plasma approximation or local-(electron) density approximation (LDA). In this model each volume element of the target atom at position $\mathbf{r}$ is considered to be an independent plasma of uniform density $\rho=\rho(\mathbf{r})$, which is equal to the electron charge density of the atom. [We normalize the density to the total number of electrons in the atom: $\int d\mathbf{r}\rho(\mathbf{r})=Z_2$.]

The electronic energy loss of a particle of charge Z_1 moving with velocity v in an electron gas of density $\rho(\mathbf{r})$ is [20]

$$-\frac{dE}{dx}(\mathbf{r})=\frac{4\pi Z_1^2}{v^2}\rho(\mathbf{r})L(\rho(\mathbf{r}),v), \tag{4}$$

where $L(\rho(\mathbf{r}),v)$ is the usual stopping number. Then the average deposited energy for a certain ion trajectory can be calculated as a linear integral of (4) along the trajectory:

$$\overline{E}(\mathbf{b})=\frac{4\pi Z_1^2}{v^2}\int_{-\infty}^{\infty}dz\rho(\mathbf{r})L(\rho(\mathbf{r}),v), \tag{5}$$

where $\mathbf{b}$ is the impact parameter and we make use of the straight-line approximation (the z axis is chosen along the ion-beam direction $\mathbf{r}=\{\mathbf{b},z\}$). Convenient approximate expressions for calculating $L(\rho(\mathbf{r}),v)$ for a free-electron gas were suggested by Lindhard and Winther [21] within the framework of the linear-response dielectric formalism. Introducing the Fermi velocity v_F and plasma frequency ω_p for the local electron gas as $v_F(\mathbf{r})=[3\pi^2\rho(\mathbf{r})]^{1/3}$ and $\omega_p(\mathbf{r})=[4\pi\rho(\mathbf{r})]^{1/2}$, the following analytical expressions for the stopping number can be written [21]: (i) for $v\leqslant v_F$,

$$L(\rho(\mathbf{r}),v)=C(\chi)\left(\frac{v}{v_F(\mathbf{r})}\right)^3, \tag{6}$$

where

$$C(\chi)=\frac{1}{2(1-\chi^2/3)^2}\left[\ln\left(\frac{1+\frac{2}{3}\chi^2}{\chi^2}\right)-\frac{1-\chi^2/3}{1+\frac{2}{3}\chi^2}\right] \tag{7}$$

and $\chi^2=1/\pi v_F(\mathbf{r})$, and (ii) for $v\geqslant v_F$,

$$L(\rho(\mathbf{r}),v)=\ln\left(\frac{2v^2}{\omega_p(\mathbf{r})}\right)-\frac{3}{5}\left(\frac{v_F(\mathbf{r})}{v}\right)^2. \tag{8}$$

The stopping cross section may be obtained by integrating the energy loss $\overline{E}(\mathbf{b})$ over all impact parameters:

$$S=\int d^2\mathbf{b}\overline{E}(\mathbf{b}). \tag{9}$$

Similarly, the energy straggling, i.e., the second momentum of the deposited energy distribution, can be calculated within the Lindhard-Scharff model as a linear integral along the trajectory:

$$W_{LS}^2(\mathbf{b})=4\pi Z_1^2\int_{-\infty}^{\infty}dz\rho(\mathbf{r})\frac{\Omega^2(\rho(\mathbf{r}),v)}{\Omega_B^2}. \tag{10}$$

Analytical approximations for the straggling in a free-electron gas were suggested by Bonderup and Hvelplund [22]: (i) for $v\leqslant v_F$,

$$\frac{\Omega^2(\rho(\mathbf{r}),v)}{\Omega_B^2}=\frac{1}{(1+13\chi^2)^{1/2}}\left(\frac{v}{v_F(\mathbf{r})}\right)^2, \tag{11}$$

and (ii) for $v\geqslant v_F$,

$$\frac{\Omega^2(\rho(\mathbf{r}),v)}{\Omega_B^2}=1+\left(\frac{1}{5}+\frac{\chi(\mathbf{r})}{\sqrt{3}}\right)\left(\frac{v_F(\mathbf{r})}{v}\right)^2\ln\left(\frac{v}{v_F(\mathbf{r})}\right)^2, \tag{12}$$

where

$$\Omega_B^2=4\pi Z_1^2Z_2. \tag{13}$$

As it was pointed out by Besenbacher *et al.* [23], the energy straggling calculated in the Lindhard-Scharff model should be corrected for the so-called bunching effect or the spatial correlations of the collisions with electrons inside the atom that lead to stronger fluctuation in the energy loss. We have used a simple approximate expression suggested in [23] to account for the bunching corrections:

$$W^2(\mathbf{b})=W_{LS}^2(\mathbf{b})+[\overline{E}(\mathbf{b})]^2. \tag{14}$$

The total straggling may be obtained from Eq. (14) as an integral over all impact parameters

$$\Omega^2=\int d^2\mathbf{b}W^2(\mathbf{b}). \tag{15}$$

C. Calculation of the ionization cross section

Given the mean deposited energy and straggling for a certain impact parameter, the probability of multiple ionization can be obtained by a convolution of the probability (1) with the deposited-energy distribution [14]:

$$P_n^{(N)}(\mathbf{b})=\int dE_T'P_n^{(N)}(E_T')w(E_T',\mathbf{b}). \tag{16}$$

Then the total cross section of multiple ionization is

$$\sigma_n = \int d^2\mathbf{b} P_n^{(N)}(\mathbf{b}). \tag{17}$$

As we have found by numerical calculations, the particular functional form of the normalized energy distribution $w(E_T', \mathbf{b})$ is not crucial for the final results provided the parameters of the distribution are fitted to give the correct value of mean energy loss and straggling. For ion-atom collisions the energy-loss spectra should decrease according to a power law in the limit of high excitation energies. This behavior is due to the root discontinuity of the electronic wave functions in the presence of a *single* Coulomb center (cf. [24,25]). As a particular functional form we have chosen the parametrization

$$w(E_T, \mathbf{b}) = N \frac{E_T^n}{(E_T + E_0)^\alpha}, \tag{18}$$

where N is a normalization factor

$$N = \frac{\Gamma(\alpha) E_0^{\alpha-n-1}}{\Gamma(\alpha-n-1)\Gamma(n+1)}, \tag{19}$$

$\Gamma(x)$ denotes the gamma function, and n, E_0, and α are the fitting parameters that are fitted to give the correct value of mean energy loss and straggling for each impact parameter (for the power $n \geqslant 1$ the minimal possible integer value is taken and $\alpha > n+3$). The shape (18) of energy-loss spectra is very similar to the experimental observations for fast ions scattered by noble-gas atoms [26]. We note, however, that such a parametrization for the deposited-energy spectra should in principle fail in the case of ion-molecule collisions since the electronic structure of molecules is defined by at least two Coulomb centers. In such a case, the Gaussian shape of the deposited-energy distribution is expected to be preferable.

III. COMPUTATION DETAILS AND SAMPLE RESULTS

In the calculations described below, the electron density distribution $\rho(r)$ has been calculated for the ground state of the target atom in the Hartree-Fock-Slater (HFS) approximation [27]. With this density distribution, using expressions (5), (10), and (14) we have calculated the mean deposited energy and the straggling of the deposited energy as functions of the impact parameter. The HFS approximation has also been used for calculating the ionization potentials $\mathcal{E}_i$ for ions in each ionization state. The ionization potential is taken to be equal, according to the Koopman's theorem, to the binding energy of the least bound electron in the ion. The obtained values have been used for calculating the probability (1) of ionization for a given deposited energy. The constant g has been considered as a free parameter, its value being fitted to give good agreement with the experimental cross section ratios. The excitation energy of the residual ion has been ignored. In the absence of any information concerning the excitation state of the residual ion it is possible only to estimate its importance in some limiting case [16]. Our experience shows that the influence of the excitation energy can be compensated for by a proper choice of the parameter g.

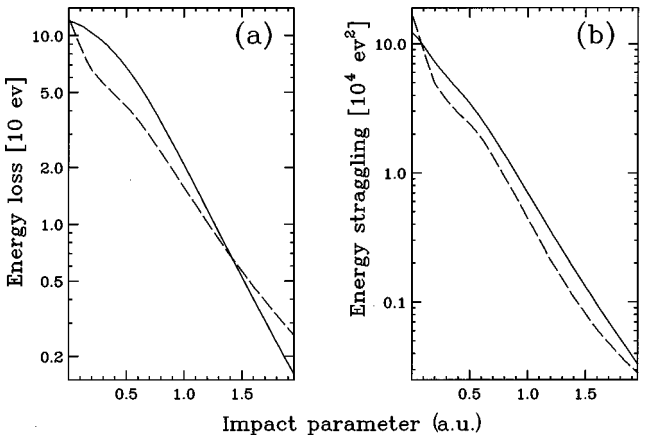

FIG. 1. Impact-parameter dependence of (a) the mean deposited energy (energy loss) and (b) the energy straggling for proton collisions with Ne atoms at the initial energy 1 MeV. Solid lines, calculations in the LDA; dashed lines, calculations in the SCA [28].

The probability of multiple ionization, differential with respect to the impact parameter, has been calculated as a convolution (16) of the probability (1) with the distribution (18) of deposited energies, characteristic for each of the impact parameters. Finally, the total cross sections for multiple ionization have been calculated by integration over all impact parameters. In the following some sample results are presented.

A. *p*-Ne collisions

The advantage of the statistical model developed is that it can be used to describe the collisions of heavy multicharged ions with heavy atoms or other multielectron targets (molecules, etc.) where no reliable theoretical methods are available. However, for illustration we first consider a much simpler example: the ionization of Ne atoms by proton impact at an energy of 1 MeV. In this case the first-order perturbation theory is applicable and the IPM is commonly assumed to be a rather good approximation for describing the double and triple ionization [6]. It is therefore interesting to compare the SED model calculations with those made by other methods. In addition, there are experimental data in abundance for this collision system.

The transferred energy and energy straggling calculated within the LDA for p-Ne collisions at $E_p = 1$ MeV are presented in Fig. 1 (solid lines) as functions of the impact parameter. We compare these results with the model calculations based on the semiclassical approximation [28] (dashed lines). The latter model, suggested in 1988 [29], is in fact an application of the SCA to the calculations of the impact-parameter dependence of electronic energy loss and straggling within the IPM. The energy loss is calculated separately for each atomic subshell and then summed over all subshells of the target atom. One can see from Fig. 1 that the two models agree reasonably well at least in the region of impact parameters around 1 a.u., which gives the main contribution to the total cross sections. At small b the LDA predicts a larger energy loss than the IPM. This leads to a somewhat larger ionization probability. At large impact pa-

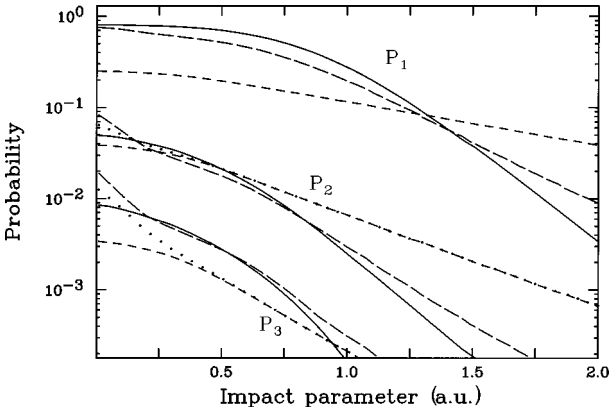

FIG. 2. Probabilities of single, double, and triple ionization of Ne atoms by 1-MeV proton impact as functions of the impact parameter. Solid curves, calculations within the SED-LDA model; long-dashed curves, SED-SCA model; short-dashed curves, IPM-SCA model (see the text for explanations); dotted curves, IPM-SCA calculations corrected for the contribution of *K*-shell Auger transitions.

rameters the LDA model strongly underestimates the mean energy loss. However, here the energy deposition is very small and can hardly influence multiple ionization. The integrated energy loss computed within the LDA agrees well with the experimental data. Here we note that the SCA calculations for Ne are probably not very reliable. At least for lower energies ($E_p = 100$ keV) the impact-parameter dependence of energy loss and straggling calculated within the SCA [28] has failed to describe accurately the experimental data [26]. For heavier noble-gas atoms Ar, Kr, and Xe the agreement is much better. At the same time the LDA calculations agree better with the SCA for heavier atoms [28].

Figure 2 shows the calculated probability of single, double, and triple ionization of Ne by proton impact as a function of the impact parameter. For each ionization state three different models are compared. The solid curves show the results of calculations within the statistical energy-deposition model with energy deposition calculated in the LDA (see the solid curves in Fig. 1). We label this result the SED LDA. The long-dashed curves show the results of SED calculations also, but with the energy deposition calculated with the SCA model (dashed curves in Fig. 1). Finally, the short-dashed curves are the results of calculations within the IPM [3]. These latter curves are very close to the results of analogous calculations by Ben-Itzhak *et al.* [6]. The only difference is that we calculated the single-particle-ionization probabilities with the HFS wave functions of Ne, whereas in [6] the scaled hydrogenic results of [30] were used. The results of the IPM have been corrected for the contribution of Auger decay of the *K*-shell vacancy, which, in principle, is included in the SED type of calculations. The corrected results are shown by the dotted curves that coincide with the short-dashed curves at the impact parameters $b > 0.5$ a.u. The comparison of the results shows that qualitatively the SED calculations agree with the IPM results. However, the SED model predicts probabilities that are larger at small impact parameters and decrease more steeply with increasing impact parameter. Qualitatively, a steeper behavior of the SED results is a consequence of a correct allowance within the SED model for an increasing ionization potential for higher charged states of the target atom.

TABLE I. Total cross sections (in 10^{-17} cm^2) for multiple ionization of Ne by 1-MeV proton impact.

	IPM	SED SCA	SED LDA	Expt.[a]
σ_1	6.0	5.0	6.3	5.7 ± 0.6
σ_2	0.22	0.14	0.14	0.13 ± 0.02
σ_3	0.012	0.019	0.017	0.004 ± 0.002

[a]Reference [31].

The total cross sections calculated within the three models described are presented in Table I together with the experimental data [31]. The agreement of calculations for the singly and doubly ionized states with the experiment is rather good. The cross section for triple ionization is overestimated by all three models. Note, however, that earlier measurements [32] gave higher cross sections close to theoretical values. We remind that in SED calculations there is a free parameter g that we have chosen to be $g = 0.01$ in all discussed results.

Concluding this subsection, we note that the SED calculation for this simple case gives similar results to the conventional IPM with the single-electron-ionization probability calculated within the SCA and agrees well with the experiment.

B. F^{4+}-Ne collisions

Our second example is the multiple ionization of Ne atoms by F^{4+} ions at 1 MeV/amu. In this case an application of the IPM with single-particle probabilities calculated in perturbation theory is at least questionable because the probability of ionization is not small.

We calculated the multiple-ionization probabilities and the cross sections within the SED-LDA model with one additional assumption. We supposed that the F^{4+} ion can be considered as a point charge $Z_1 = 4$. The radius of the F^{4+} ion is about 0.2 a.u.; therefore, at least for impact parameters larger than 0.2 a.u. this should be a reasonable approximation. Below (see Sec. IV) we discuss the possibilities to improve the calculations and to account for the dimension of the projectile electron cloud.

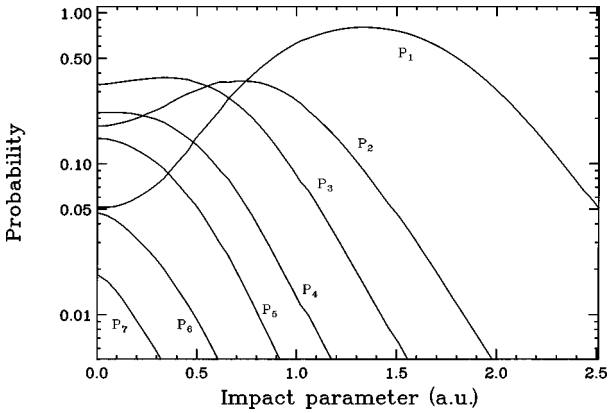

FIG. 3. Probabilities of multiple ionization of Ne atoms in collisions with 1-MeV/amu F^{4+} ions as a function of the impact parameter, calculated within the SED-LDA model.

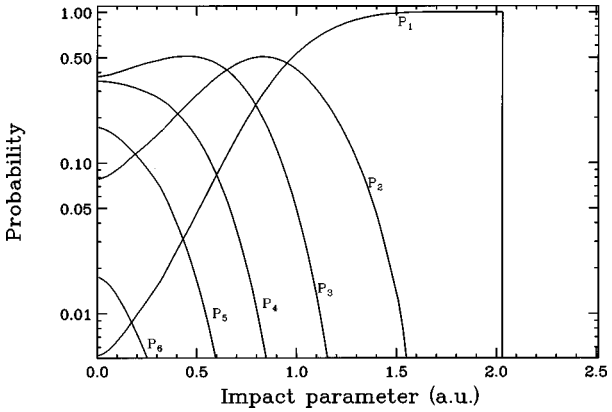

FIG. 4. Same as in Fig. 3, but calculated disregarding the straggling of the deposited energy.

Figure 3 shows the probabilities of multiple ionization as functions of the impact parameter. Qualitatively, our results are similar to the results obtained for the Ne^{10+} + Ne collisions in the IPM [9,6] and for the Cl^{9+} + Ne collisions in the SED model [16]. The probability functions are peaked at different values of b. At least for single, double, and triple ionization the contributing impact parameter ranges are somewhat different, forming windows in impact-parameter space for the various degrees of multiple ionization. For higher stages of ionization the distributions are peaked at $b=0$. Note that in our model the windows are broader than in the IPM calculations [6] and early SED calculations [16]. This may be partly explained by a large straggling of the deposited energy. To illustrate this statement and to demonstrate the role of the energy straggling in forming the profile of the probability function, we show in Fig. 4 the results similar to Fig. 3, but calculated disregarding straggling ($\Omega^2=0$). Evidently, the windows are now more pronounced; the single-ionization probability increases stepwise at about $b=2.0$ a.u., where the energy loss has become equal to the first-ionization threshold.

In Fig. 5 the calculated multiple-ionization cross sections (normalized to the single-ionization cross section) are compared with the experimental data [33]. The overall agreement is very good. The single-ionization cross section obtained in the SED-LDA model is 2.32×10^{-16} cm^2, in reasonable agreement with the measured one, $(4.3\pm1.3)\times10^{-16}$ cm^2. In the calculations for the F^{4+} case the parameter g was taken to be $g=0.012$, which is close to the value obtained for the p+Ne case.

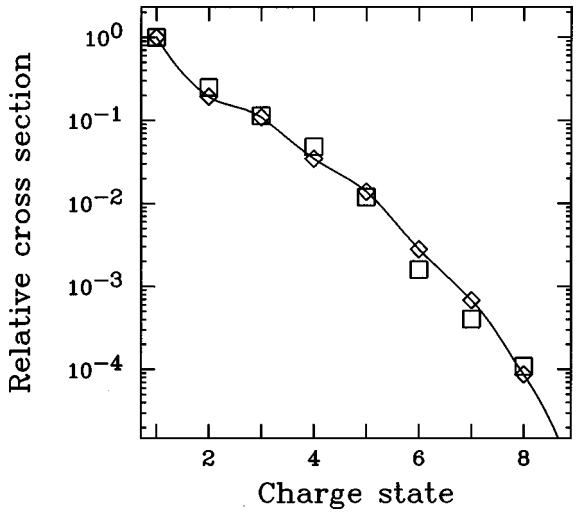

FIG. 5. Cross sections for multiple ionization of Ne atoms for 1-MeV/amu F^{4+} ion impact. Diamonds connected by lines, SED-LDA calculation; squares, experimental data from [33].

IV. CONCLUSION

We have described an extended version of the statistical energy-deposition model and demonstrated its applications to multiple ionization in fast ion-atom collisions. Using the LDA for the calculation of the energy transfer and the statistical distribution of the transferred energy, we obtained a realistic description of this process. For the case of p-Ne collisions in the domain of the SCA, our model compares favorably with the IPM results and agrees well with experiment. It turns out to be adequate also in the more complex case of F^{4+}-Ne collisions. Thus we can conclude that the SED-LDA model can serve as a good tool in studying fast ion-atom collisions.

Our main goal, however, was to suggest a model that can be easily extended to ion collisions with more complicated structures: molecules, clusters, etc. This goal has been accomplished by introducing the local-density approximation for calculating the energy deposition. In this approximation the target is characterized by the ground-state electron density only. Therefore, this approach can be easily extended to the case of ion-molecule collisions provided the electron density of the target molecule is known. We plan to present an application of the model to multiple ionization of molecules in our next paper [19].

The model developed suggests several other possibilities. For example, it is easy to consider the differential cross sections of various multiple-ionization channels. In fact, in the lower-energy range the SED model was already applied to a description of differential cross-section measurements [13]. Using the model described above, one can easily calculate the differential cross section by transforming the impact-parameter-dependent probability into the scattering-angle-dependent cross section. Such calculations could be interesting for the interpretation of recent experimental data at high energies [34].

Another important generalization that can be easily done within the SED-LDA model is studying the ionization produced not by ''bare'' structureless particles but by ions carrying their own electrons that effectively screen the nuclear charge. The screening effect, which is impact parameter dependent, can be easily incorporated into the developed scheme of calculations using the modification of the LDA method suggested by Ferrell and Ritchie [35] and by Brandt and Kitagawa [36] (see also [37] and references therein).

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