

Precise charge-state distribution of projectile ions through solid targets

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The charge-state distribution (CSD) of the projectile ions through solid targets in the intermediate energy range ($1 \text{ MeV/u} < E < 4 \text{ MeV/u}$) has a major impact on the collision of the ion atom and accelerator physics. We explore the mean charge states taken from the empirical formula [G. Schiwietz *et al.*, *Femtosecond dynamics—snapshots of the early ion-track evolution*, *Nucl. Instrum. Methods Phys. Res., Sect. B* **225**, 4 (2004)] are only good for projectile ions with $Z_1 \leq 16$. To solve this issue, we develop a model in which instead of a single formula, if we employ four formulas, the comparative picture between experimental and empirical data becomes impressive. Furthermore, the CSDs obtained using the mean charge state and the Gaussian distribution function having distribution width as given by Novikov and Teplove [Methods of estimation of equilibrium charge distribution of ions in solid and gaseous media, *Phys. Lett. A* **378**, 1286 (2014)] show good agreement with the experimentally measured CSDs for the entire range of projectile ions. We believe that accurate CSDs will be highly useful for both ion-atom collision and accelerator physics.

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I. INTRODUCTION

When a monochromatic focused ion beam with a particular initial charge state (q) passes through a solid target, it undergoes atomic excitation and ionization processes. As a result, the projectile ion loses some of its kinetic energy inside the target, and this energy loss depends on the kinetic energy of the ion beam, the atomic numbers of the projectile (Z_1), the target (Z_2) and the initial charge state of the projectile ions. Consequently, it results in a rapid change in the projectile charge state inside the target (q_m^i). Subsequently, the projectile ions with q_m^i interact with the target surface layers at emerging energy, which experience profound charge exchange [1]. This causes a change in the charge state from q_m^i to the charge state of the projectile ions after passing through the target foil (q_m^o) [1]. Note that the plasma medium is even better charge stripper than the solid targets. Therefore, q_m^i is normally higher than q_m^o [2–4] because the initial charge state of the projectile ions pass through the beam-foil plasma [5] formed inside the foil

by ion-solid interactions. On the contrary, projectile ions with q_m^i have to pass through the exit layers of the target foil from where the quasi-free electrons present at the surface of the foil can easily jump to the projectile ions. The q_m^o and the charge-state distribution (CSD) of the emerging projectile ions are accurately measured by standard electromagnetic methods [6].

The prediction of q_m^o is also performed by empirical models if q_m^o is reached to charge equilibrium. When we consider charge equilibrium cases, the initial charge state of the projectile ions does not play any role in estimating the q_m^o and CSD if the initial charge states are not H-like or bare ions [7]. Many empirical models [8–13] have been used to obtain such an equilibrated q_m^o . Of these models, the Schiwietz and Grande [10] model defined q_m^o as follows:

$$q_m^o = Z_1 \frac{12x_{01} + x_{01}^4}{0.07/x_{01} + 6 + 0.3x_{01}^{0.5} + 10.37x_{01} + x_{01}^4}, \quad (1)$$

where x_{01} is a reduced parameter given by

$$x_{01} = (v_1/v_o Z_1^{-0.52} Z_2^{-0.019 Z_1^{-0.52} v_1/v_o / 1.68})^{1+1.8/Z_1}. \quad (2)$$

Let us call this model SGM, which is often used for the prediction of q_m^o : for example, see Refs. [3,4,14]. Subsequently, it was further improved by the same group [9], we call it improved SGM (ISGM). Although it improved q_m^o to a good extent. However, it did not describe CSD at all. If we consider the distribution width (Γ) of Schiwietz and

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Grande [10] is valid here also, but that formula contains a charge-state fraction $[F(q)]$ term as follows:

$$\Gamma = \left[\sum_q (q - q_m^o)^2 F(q) \right]^{1/2}. \quad (3)$$

Usually, Γ should be independent of $F(q)$, so $F(q)$ can be defined as a function of q_m^o and Γ . However, here $F(q)$ is used in Eq. (3) for obtaining Γ , which implies that $F(q)$ must be taken only from the experimental data. Thus, both SGM and ISGM cannot predict $F(q)$ and without $F(q)$, the charge-state distribution cannot be obtained. Hence, neither SGM nor ISGM can predict CSD, which is highly essential for many practical applications. Although theoretical models such as ETACHA [7,14–16], CHARGE (a three-state model), and GLOBAL (a 28-state model) [17] have been developed to obtain CSD to simulate charge exchange dynamics, they also have limitations. ETACHA [7,14–16] works effectively for intermediate and high-energy regimes [16] but struggle with heavy ions that have more electrons than Ni-like ions. CHARGE and GLOBAL [17], on the other hand, are primarily designed for high-energy relativistic ions, leaving a gap in the prediction of charge-state distributions for the intermediate energies. These limitations require a reconsideration of earlier empirical models and exploration of a new approach to obtain CSD independently (without requiring any assistance from experimental charge-state fractions).

Heavy ions with intermediate energies are quite easy to produce and are very useful for accelerator applications, as heavy ions in the intermediate energy range are used to pass through the charge stripper to have higher charge states, so higher energy will be obtained from the booster stage of the large accelerators. On this ground, empirical formulas may prove useful if we find a way to generate CSD using the estimated values of q_m^o . Normally, q_m^o is the center point of the CSD, which means that the highest $F(q)$ is obtained at the rounded value of q_m^o . However, during practical applications, a full CSD curve is very essential if an accelerator has to use any other charge states to obtain an ion beam of the required energy for a certain application. Hence, a methodology for estimating the $F(q)$ without limitations is extremely important. In this respect, empirical models find their worth.

To estimate the CSD, there are many empirical models in the literature [8,18,19]. These models used q_m^o and Γ in the Gaussian distribution to obtain the charge-state fraction. Different formulas are used to obtain the correct q_m^o for different regions of the atomic numbers of the projectile [8]. To eliminate such difficulties, Schiwietz and Grande [10] and Schiwietz *et al.* [9] formulated a single formula to empirically calculate q_m^o for the entire range of projectiles and targets.

In this work, we attempt to estimate (i) q_m^o in good agreement with the experimental values, (ii) the distribution

width close to the experimental figures, and (iii) finally $F(q)$ and CSD in accordance with the experiments so that these estimated values can be used in different fundamental and practical applications. We present here the methodologies and other details.

II. CHARGE-STATE DISTRIBUTION OF THE PROJECTILE ION OUTSIDE THE TARGET FOIL

Of several models mentioned above, the Schiwietz Grande Model (SGM) [10] was used mainly to predict the mean charge state (q_m^o) because a single formula worked for the entire range of projectile ions on solid target foils. However, it often does not represent the experimental scenario. Consequently, the same group developed an improved formula (ISGM) [9]. We used ISGM to calculate q_m^o . According to ISGM, q_m^o is expressed as a function of a reduced parameter x_{02} and the projectile atomic number Z_1 as follows:

$$q_m^o = \frac{Z_1(8.29 x_{02} + x_{02}^4)}{\frac{0.06}{x_{02}} + 4 + 7.4 x_{02} + x_{02}^4}. \quad (4)$$

Here, the reduced parameter x_{02} is written in terms of projectile velocity (v_1), projectile atomic number Z_1 , and target atomic number Z_2 as follows:

$$x_{02} = c_1 \left(\frac{\bar{v}}{c_2 \cdot 1.54} \right)^{(1 + \frac{1.83}{Z_1})}, \quad (5)$$

$$\bar{v} = Z_1^{-0.543} \left(\frac{v_1}{v_o} \right), \quad (6)$$

$$c_1 = 1 - 0.26 \exp \left(-\frac{Z_2}{11} \right) \exp \left(-\frac{(Z_2 - Z_1)^2}{9} \right), \quad (7)$$

$$c_2 = 1 + 0.030 \bar{v} \ln(Z_2), \quad (8)$$

where v_o is the Bohr velocity (2.19×10^6 m/s). Next, the distribution width Γ is taken from Novikov and Teplova [20] (NAT) as

$$\Gamma(x_1) = C[1 - \exp(-(x_1)^\alpha)][1 - \exp(-(1 - x_1)^\beta)], \quad (9)$$

where x_1 is given as

$$x_1 = q_m^o/Z_1 \quad (10)$$

and $\alpha = 0.23$, $\beta = 0.32$, $C = 2.669 - 0.0098 \cdot Z_2 + 0.058 \cdot Z_1 + 0.00048 \cdot Z_1 \cdot Z_2$.

Next, we have compared the mean charge state q_m^o as obtained from Eq. (4) (ISGM [9]) and the width of the charge-state distribution $\Gamma(x_1)$ [Eq. (9)] from Novikov and Teplova [20] (NAT) with the corresponding experimental data [13,21] as a function of the energy of emergence in Fig. 1. The exit energy is estimated by deducting the ion

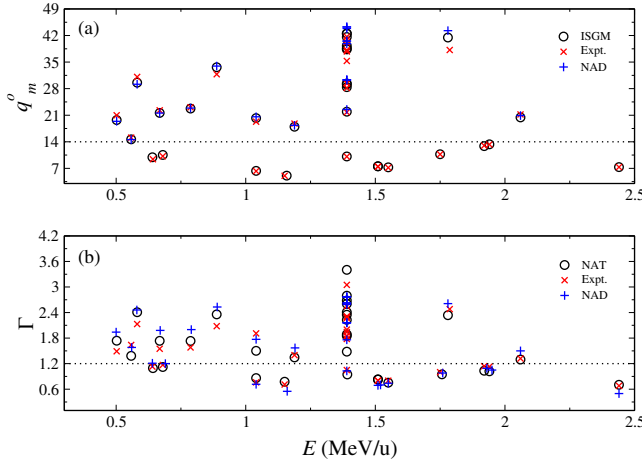


FIG. 1. (a) Projectile mean charge state (q_m^o) versus beam energy [E (MeV/u)]: Comparison of experimental q_m^o (red cross) [13,21] with the empirical q_m^o using ISGM [Eq. (4)] (black circle) [9] and NAD [Eq. (11)] (blue plus) [19]. (b) Distribution width (Γ) versus beam energy [E (MeV/u)]: Comparison of experimental Γ (red cross) [13,21] with empirical Γ using NAT [Eq. (9)] (black circle) [20] and NAD [Eq. (13)] (blue plus) [19]. Projectile-target combinations are as follows: C, O, F, Si, Cl, Cu, Kr, Xe, Au, Pb, and U ions on C; F, Xe, and U on Al; Si and Pb on Ag; F, Xe, and U on Au; Si on Pb; Cl on Ni and Bi from Shima *et al.* [13]; Ag ions on C target from Ball *et al.* [21].

energy loss in the foil calculated using the SRIM package [22] from the incident beam energy. Here, one can see that both these q_m^o [Eq. (4)] and $\Gamma(x_1)$ [Eq. (9)] agree well with the experimental data for the heavy ions up to $Z_1 = 16$. However, the picture is not the same for the heavy ions $Z_1 > 16$. To check whether the Nikolaev and Dmitriev [19] (NAD) formula for predicting the mean charge state of projectile ions through solid targets (q_m^o) fits better, we have used q_m^o ($Z_1 > 16$) as

$$q_m^o = Z_1 [1 + (Z_1^{-0.45} v_1 / v')^{-1/0.6}]^{-0.6} \quad (11)$$

Here $v' = 3.6 \times 10^8$ cm/sec.

In addition to the above formula, many other formulas that work for different Z_1 are also given in the review of BETZ [8]. The agreement of q_m^o in ISGM (black) [9] and NAD (blue) [19] with the experimental mean charge state [13,21] of projectile ions through solid targets (red cross) seems to look quite similar in Fig. 1. To examine which one agrees better in this comparison, we have evaluated the data using a quantity called the relative sum of squares error (RSSE). RSSE is just the sum of squared errors (SSE = $\sqrt{\sum_i^n [y_i - f(E_i)]^2}$) divided by the sum of the experimental values (y_i) as follows:

$$\text{RSSE} = \frac{\sqrt{\sum_i^n [y_i - f(E_i)]^2}}{\sum_i^n y_i}, \quad (12)$$

where $f(E_i)$ is the theoretical counterpart of y_i . Comparison of the RSSE of q_m^o for all the projectile-target systems considered in Fig. 1 with reference to the two models shows that ISGM [9] gives an RSSE of 0.010 while NAD [19] shows an error of 0.018.

The distribution width Γ for different projectiles Z_1 is given by Nikolaev and Dmitriev [19] as follows:

$$\Gamma = 0.5 [q_m^o (1 - (q_m^o / Z_1)^{1/0.6})]^{1/2}. \quad (13)$$

Using q_m^o from Eq. (4), we further tested the case of two distribution widths of NAT [20] and NAD [19]. We found that Eq. (9) or $\Gamma(x_1)$ of Novikov and Teplova [20] gives an error of 0.023 and Eq. (13) or NAD has an error of 0.028. Hence, we used ISGM [9] for q_m^o [Eq. (4)] and NAT [20] for distribution widths [$\Gamma(x_1)$] taken from Eq. (9).

Next, to get the charge-state fractions ($F(q)$), we have used the Gaussian charge-state distribution [13] as

$$F(q) = \frac{1}{\sqrt{2\pi}\Gamma} \exp(-(q - q_m^o)^2 / 2\Gamma^2) \quad (14)$$

provided

$$\sum_q F(q) = 1. \quad (15)$$

However, Shima *et al.* [13] used three different distributions— χ^2 , Gaussian, and reduced χ^2 —for CSD at low, intermediate, and high charge states of projectile ions, respectively. In Fig. 2, we have compared the Gaussian charge-state distribution for the entire range of charge states (low, intermediate, and high) with the three distributions for Ar ions on the carbon target, as shown in Shima *et al.* [13].

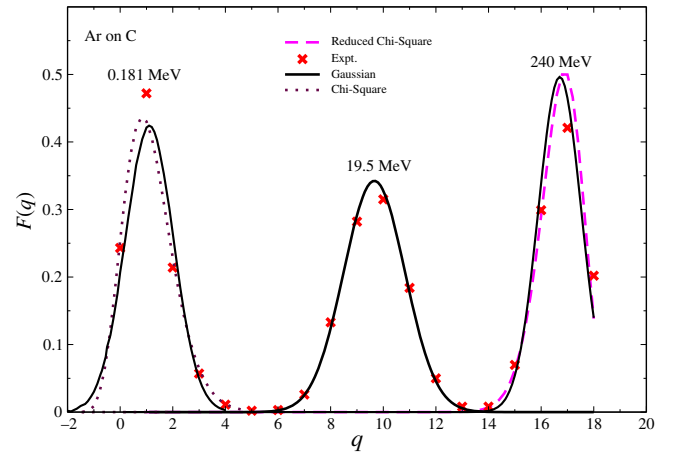


FIG. 2. Charge-state distribution (CSD) curve of Ar ions on carbon target foil (charge-state fraction [$F(q)$] versus charge state (q)): Comparison of the experimental CSD (red cross) with χ^2 distribution (dotted maroon) for low charge Ar ions, reduced χ^2 distribution (dash pink) for high-charge Ar ions, and Gaussian distribution (black) for entire charge range of Ar ions.

We examined the goodness-of-fit for all distributions using a measure of RSSE studies. The RSSE of the Gaussian distribution turns out to be 0.0803, 0.0204, and 0.000087 for low, intermediate, and high charge states of Ar ions on C targets, respectively. The RSSE is 0.0466 and 0.000101 for the χ^2 (low charge) and reduced χ^2 (high-charge) distributions, respectively. It implies that the χ^2 distribution for low charge is certainly better than the Gaussian charge-state distribution curve with q_m^o from ISGM [9] or Eq. (4) and $\Gamma(x_1)$ from Eq. (9) in fitting the experimental data [13,21]. However, the latter is good not only for intermediate-charge Ar ions but also for high-charge Ar ions. Hence, the use of $\Gamma(x_1)$ from Eq. (9) in the Gaussian charge-state distribution curve [Eq. (14)] may address both intermediate and high-charge projectile ions well.

III. PROBLEM ARISES WITH ISGM q_m^o

To test the above-mentioned methodology, different projectile ($Z_1 \leq 17$) target systems at various energies have been shown in Fig. 3. We see that the empirical formula for $F(q)$ fits well with the experimental data [13,21] except for

two cases (i) and (l). In both cases, Cl is the projectile, while carbon and bismuth are the targets in (i) and (l), respectively. Note that Cl is the heaviest projectile of all the projectiles used in this figure. Four cases with the Cl projectile (i)–(l), (j) and (k) are also shown with different targets of carbon and nickel, respectively, but with higher beam energies. In contrast, (i) and (l) are done with lower beam energies. Furthermore, in Fig. 1, we have already mentioned that q_m^o is not good for heavy ions. Hence, the reason for the disagreement in CSD is both the low beam energy and heavier projectiles.

To clarify the above-mentioned doubts, we have investigated the heavy-ion cases in Fig. 4. Except for a few cases in Figs. 4(h), 4(i), and 4(k), the other 17 datasets show a clear mismatch between the empirical and experimental CSD. To find the real cause of this disagreement, we employed the same method using $\Gamma(x_1)$ from Eq. (9) and the Gaussian charge-state distribution from Eq. (14), but the mean charge state of the projectile ion is taken from experimental data [13,21]. Using this technique, we found good agreement between the empirical (green curve) and experimental (red cross) charge-state distribution even with

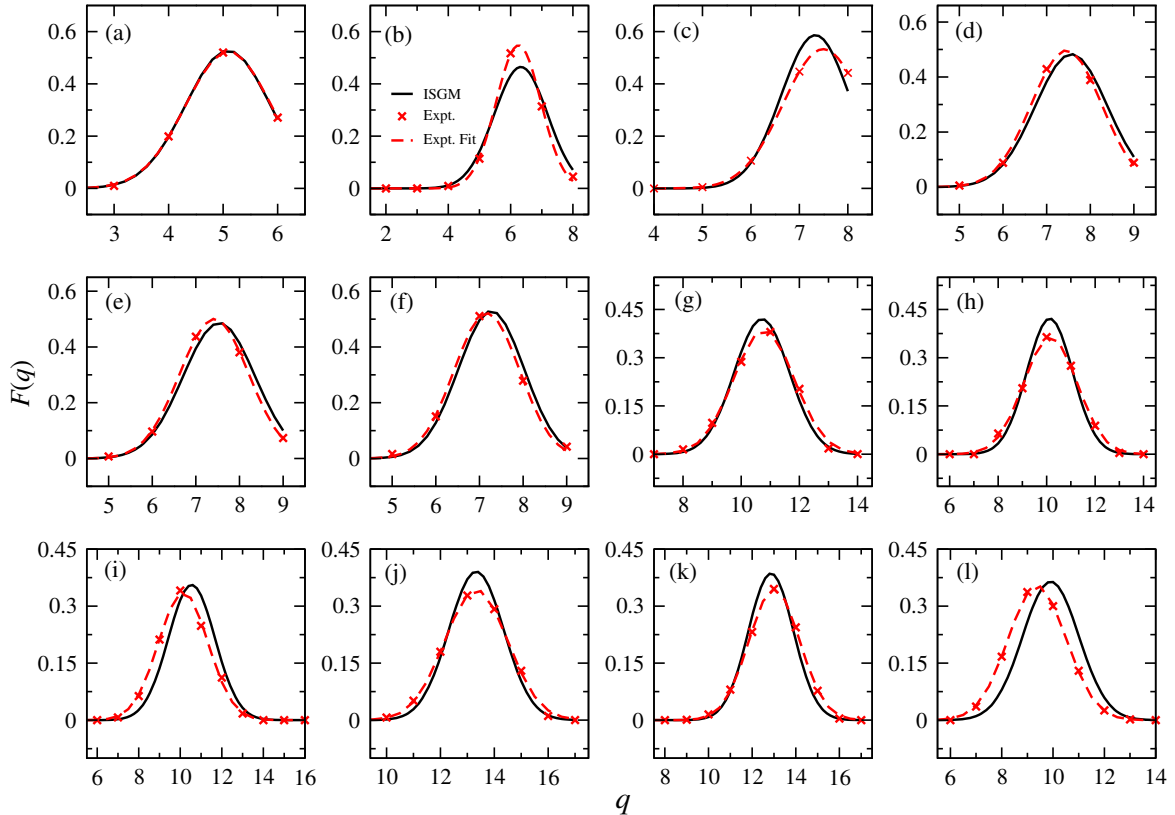


FIG. 3. Gaussian charge-state distribution (CSD) curves with solid black line are plotted using Eqs. (4), (9), and (14) for different projectile ions ($Z_1 \leq 17$) and various solid targets at diverse energies to compare with the corresponding experimental data [13] shown with red cross. The experimental data are further fitted with red dashed line for clarity. (a) C on C (1.158 MeV/u), (b) O on C (1.04 MeV/u), (c) O on C (2.44 MeV/u), (d) F on C (1.510 MeV/u), (e) F on Al (1.515 MeV/u), (f) F on Au (1.552 MeV/u), (g) Si on Ag (1.757 MeV/u), (h) Si on Pb (1.392 MeV/u), (i) Cl on C (0.688 MeV/u), (j) Cl on C (1.948 MeV/u), (k) Cl on Ni (1.925 MeV/u), and (l) Cl on Bi (0.642 MeV/u).

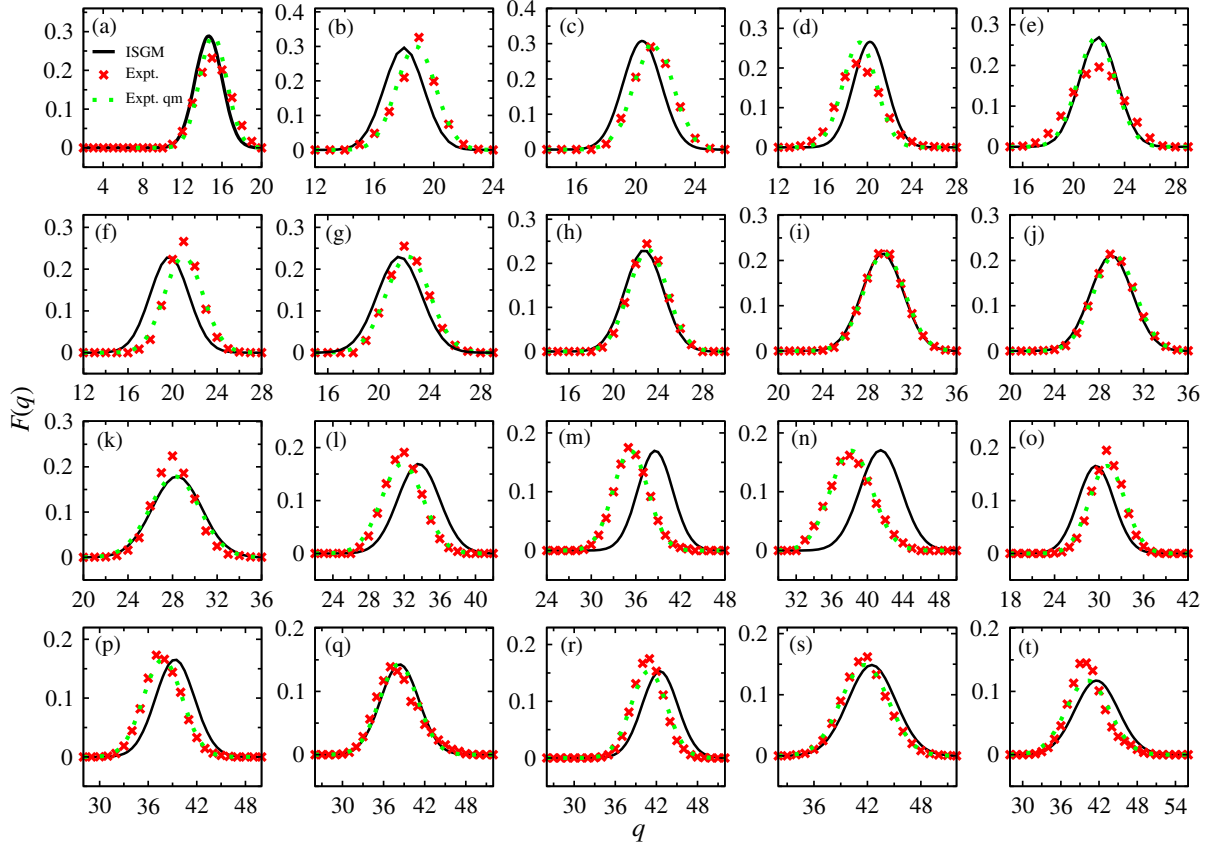


FIG. 4. Gaussian charge-state distribution (CSD) curves with the distribution width from NAT [20] [Eq. (9)] for different projectile ions ($Z_1 > 17$) and various solid targets at diverse energies using q_m^o from (i) ISGM [Eq. (4)] (black) [9] and (ii) experiments (green) [13,21] are compared with the corresponding experimental results. Experimental data for Ag ions on C target (f)–(h) are from Ball *et al.* [21]; all other projectile-target systems are from Shima *et al.* [13]. (a) Cu on C (0.558 MeV/u), (b) Cu on C (1.188 MeV/u), (c) Cu on C (2.060 MeV/u), (d) Kr on C (1.04 MeV/u), (e) Kr on C (1.39 MeV/u), (f) Ag on C (0.502 MeV/u), (g) Ag on C (0.668 MeV/u), (h) Ag on C (0.787 MeV/u), (i) Xe on C (1.39 MeV/u), (j) Xe on Al (1.39 MeV/u), (k) Xe on Au (1.39 MeV/u), (l) Au on C (0.888 MeV/u), (m) Au on C (1.396 MeV/u), (n) Au on C (1.786 MeV/u), (o) Pb on C (0.581 MeV/u), (p) Pb on C (1.39 MeV/u), (q) Pb on Ag (1.39 MeV/u), (r) U on C (1.39 MeV/u), (s) U on Al (1.39 MeV/u), and (t) U on Au (1.39 MeV/u).

low beam energies. Hence, there is no issue with the proposed empirical formulation as far as the distribution width and Gaussian distribution are concerned in representing the experimental charge-state distributions. Our challenge remains to evaluate the mean charge state outside the foil well for the heavier ions ($Z_1 \geq 17$). The next attempt was to find the mean charge state also empirically instead of experimental ones. A thorough search shows that the mean charge state obtained from Schiwietz *et al.* [9] agrees well with the experimental results if $Z_1 \leq 16$, but the scenario is not so for $Z_1 > 16$, as we see from the above results. So far, this work concludes that the challenge of an empirical formula for evaluating the mean charge states outside the target foil is not yet over. Hence, to improve q_m^o empirically, we proceed far to solve this problem.

IV. RENEWED FORMULAS FOR q_m^o

The improvement of ISGM from SGM was achieved by introducing a different reduced parameter x_{02} instead of x_{01} .

To investigate the role of the reduced parameter in the mean charge-state formula, we examined the relationship between the reduced parameter and the normalized charge state q_m^o/Z_1 for both the SGM (x_{01}) and ISGM (x_{02}) models in Fig. 5. The parameter x_{01} for SGM [10] is given in Eq. (2) while Eq. (5) stands for the ISGM reduced parameter x_{02} .

We revealed that Fig. 5(a) exhibits a distinctive four-band pattern in the data, which is not observed in Fig. 5(b). Exactly, this was the objective of ISGM. However, this upgrade did not work well, so we decided to use the earlier x_{01} , from different points of view, as defined in the SGM [Eq. (2)] from this instance.

The reason for this consideration of the parameter x_{01} is quite clear from Fig. 5(a); the data constitute a widespread band, and a single fitted line is too simple to provide fairness to such data. Furthermore, we notice that projectiles on heavier targets ($Z_2 > 6$) particularly widen the width of the curve. To avoid such a problem, we first consider only the experimental data on the light (carbon) targets, which can be classified into four groups of projectile ions as follows: (a)

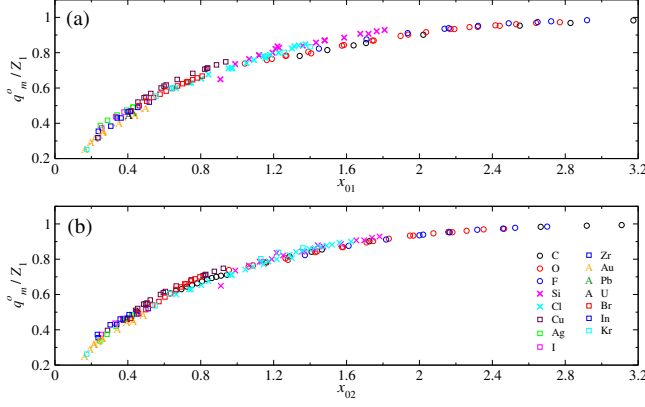


FIG. 5. Experimental q_m^o/Z_1 versus x_{01} or x_{02} plot: the reduced parameter x_{01} [Eq. (2)] and x_{02} [Eq. (5)] are taken from Schiwietz and Grande [10] for (a) and Schiwietz *et al.* [9] for (b). Experimental q_m^o data for different projectiles on carbon targets are taken from Refs. [13,21].

$4 \leq Z_1 \leq 10$, (b) $11 \leq Z_1 \leq 18$, (c) $19 \leq Z_1 \leq 54$, and (d) $55 \leq Z_1 \leq 92$. The q_m^o/Z_1 are plotted as a function of the same reduced parameter x_{01} , as given in Eq. (2), and all four curves in Fig. 6 have been fitted with the standard logistic function as follows:

$$\frac{q_m^o}{Z_1} = \frac{L}{1 + \exp[-K(x_o - x')]} \quad (16)$$

where x' is the value of x_o at the midpoint, L is the maximum value of $\frac{q_m^o}{Z_1}$, and K is the logistic growth rate of the curve. The q_m^o for projectile ions that fall in the range of $4 \leq Z_1 \leq 10$ is denoted by $q_{m_1}^o$ and can be obtained using the empirical formula as follows:

$$q_{m_1}^o = Z_1 \frac{1.007704}{1 + \exp[-1.419686(x_o - 0.416069)]} \quad (17)$$

Similarly, the q_m^o data for the projectile ions that fall in the range of $11 \leq Z_1 \leq 18$, $19 \leq Z_1 \leq 54$, and $55 \leq Z_1 \leq 92$ are denoted by $q_{m_2}^o$, $q_{m_3}^o$, and $q_{m_4}^o$, respectively, and can be obtained from the following empirical formulas:

$$q_{m_2}^o = Z_1 \frac{0.966005}{1 + \exp[-2.117365(x_o - 0.454663)]} \quad (18)$$

$$q_{m_3}^o = Z_1 \frac{0.901506}{1 + \exp[-2.674817(x_o - 0.368080)]} \quad (19)$$

and

$$q_{m_4}^o = Z_1 \frac{0.525255}{1 + \exp(-7.609263(x_o - 0.170544))} \quad (20)$$

There are sufficient data to fit the curve of Figs. 6(a)–6(c), but the data available for fitting the curve of Fig. 6(d) are not many. Only data exist with Au at several energies and a few points for Pb and U projectiles. In spite of this, we got a good fit, and the corresponding equation can be used for our future use. Furthermore, two data points for gold ions deviate from the fitted line; the shell effect may be one of the reasons.

In the above equations, q_m^o varies from $q_{m_1}^o$ to $q_{m_4}^o$ depending on the projectile ions. Next, to obtain the values of the charge-state fraction ($F(q)$), we have used the Gaussian charge-state distribution from Eq. (14) and $\Gamma(x_1)$ is taken from the distribution width given by Novikov and Teplova [20] [Eq. (9)]. We replace the quantity

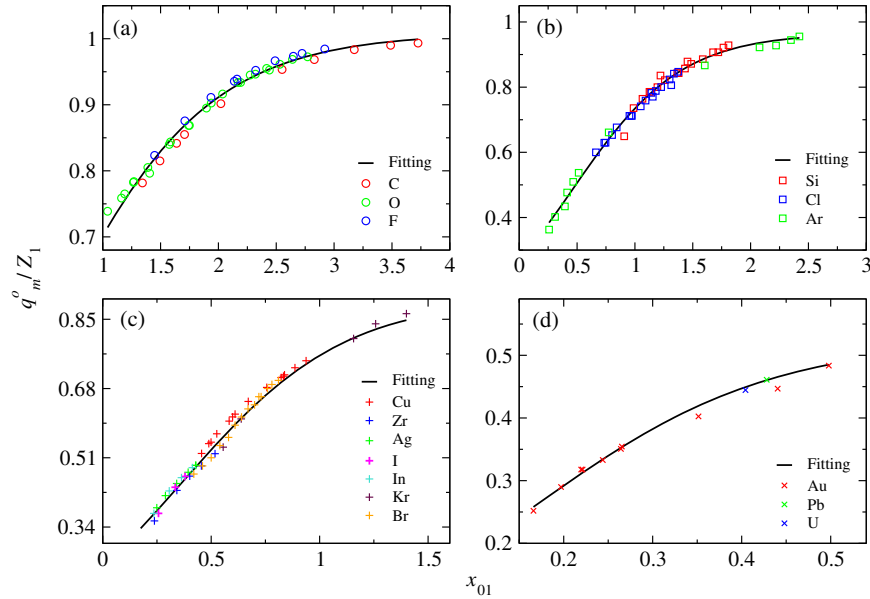


FIG. 6. Same as Fig. 5(a) but the data are divided into four groups: data for ion beams (a) $4 \leq Z_1 \leq 10$, (b) $11 \leq Z_1 \leq 18$, (c) $19 \leq Z_1 \leq 54$, and (d) $55 \leq Z_1 \leq 92$.

x_1 as used in Eq. (10) to calculate the width distribution $\Gamma(x_1)$ in Eq. (9) as follows

$$x_1 = \frac{q_m^o(m = m_1, m_2, m_3, m_4)}{Z_1}. \quad (21)$$

V. PHYSICS BEHIND DIVIDING THE FULL RANGE OF PROJECTILE IONS INTO FOUR GROUPS

We have divided the full range of projectile ions into four groups. Naturally, a basic question arises in mind as to what the physics behind such occurrences is. Incidentally, we find a certain observation during an ongoing piece of work in which we intend to check the nature of beam-foil plasmas formed under different experimental conditions. We notice indeed that the nature of beam-foil plasma does vary with the projectile-target systems even though the beam velocity is the same. The nature of beam-foil plasmas formed with oxygen and neon ions on the same target is similar, but this plasma nature is quite different from that formed by argon ions with the same targets. The mean charge state inside the target does vary with the nature of the beam-foil plasma, and the mean charge state outside the target again depends on it. Consequently, projectile ions with $Z \leq 10$ must be placed in one group and those with $Z \leq 18$ in a different group. This work is underway; a lot

more cases have to be studied to explore the relevant physics in detail. Although we are not in a position to shed more concrete light on it. Still, it gives some flavor to the readers about the physics behind classifying the entire range of projectile ions into four groups.

VI. RESULTS AND DISCUSSIONS

We have used the reduced parameter x_{01} of the SGM from Eq. (2) and the ratio of q_m^o and Z_1 plotted along the x axis and y axis, respectively, in Fig. 5(a). Then it was observed that all the data do not show the same trend. A clear difference can be seen here as we move from $Z_1 = 6$ to 92. Hence, we divide the entire existing data into four categories according to their trend and fit it accordingly in Fig. 6. This fitting gives us a clear picture to obtain q_m^o well and yields the fitting Eqs. (17)–(20) for any ion beams on the carbon target. A representative comparison of experimental q_m^o (red cross) for different ion beams on carbon target foil with SGM (dotted green), ISGM (blue dashed line), and the present model (solid black line) is presented in Fig. 7. It shows clearly that the present model best agrees with the experimental data. Furthermore, we know that ISGM is good for light ion regime $Z_1 \leq 16$. To check whether present model predictions for q_m^o in this region are even better than either SGM or ISGM, we have found out the RSSE values of SGM, ISGM, and present model for

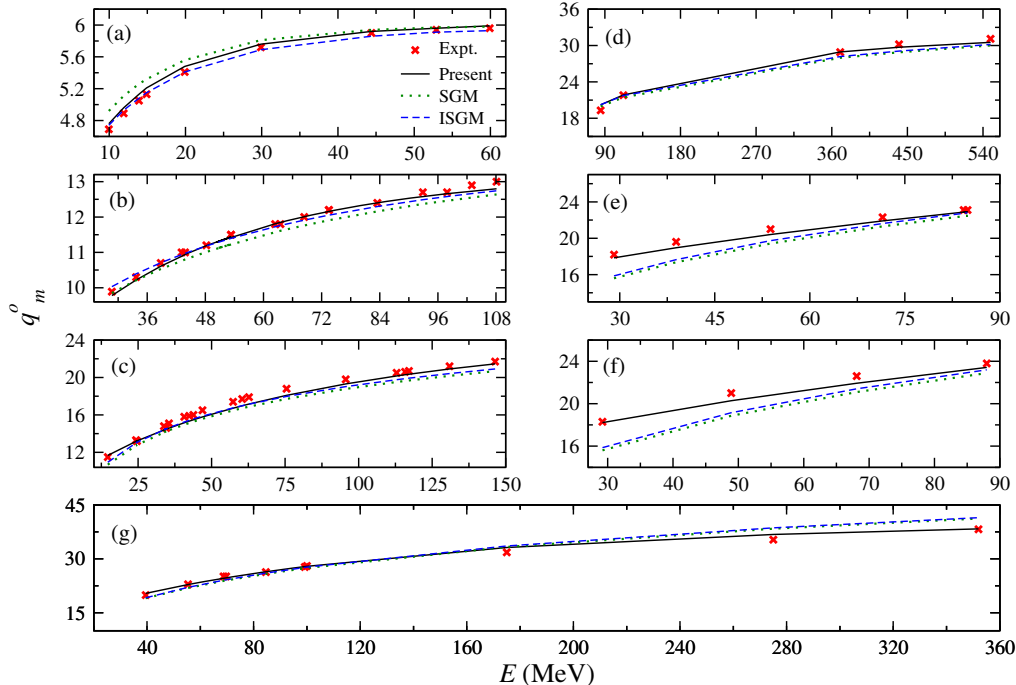


FIG. 7. Comparison of experimental mean charge states (q_m^o) of different ion beams on carbon target [13,21] with Eqs. (1) (SGM [10]) and (4) (ISGM [9]), and our model [Eqs. (17)–(20)] as a function of beam energy (E). Experimental data for the projectile ions ^{12}C , ^{28}Si , ^{63}Cu , ^{83}Kr , and ^{197}Au are taken from Shima *et al.* [13]. While the data for ^{63}Cu , ^{107}Ag , ^{114}In , and ^{197}Au ion beams are from Ball *et al.* [21]. Note that data for the projectiles ^{63}Cu and ^{197}Au are taken from both [13,21]. (a) C on C, (b) Si on C, (c) Cu on C, (d) Kr on C, (e) Ag on C, (f) In on C, and (g) Au on C.

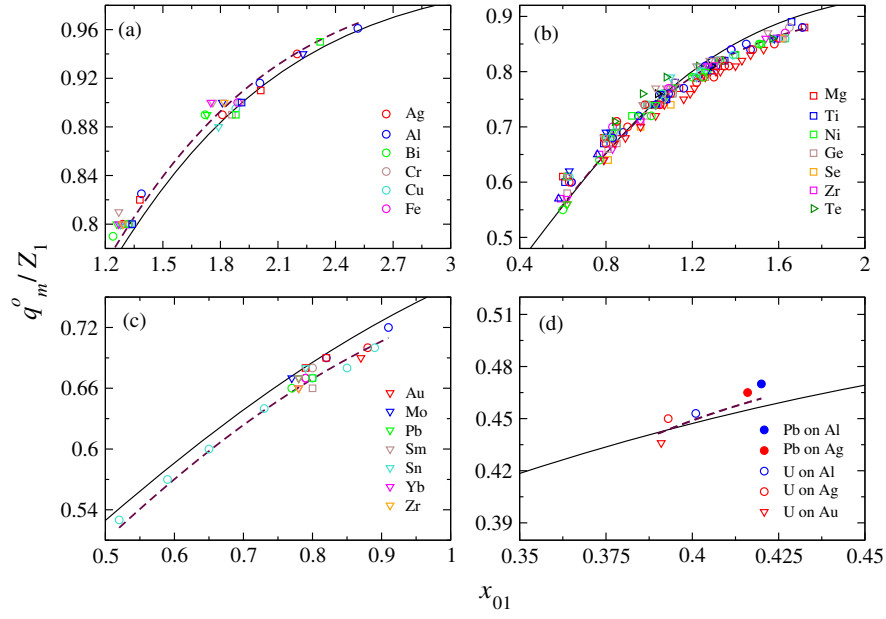


FIG. 8. Same as Fig. 6 but for miscellaneous targets excepting the carbon for different projectile ions. Solid lines represent Eqs. (17)–(20) for (a)–(d), respectively, and the dash lines is drawn with respect to the equations given in Table I. (a) F, (b) Si and Cl, (c) Cu, and (d) Pb and U.

TABLE I. Certain correction terms added with the mean charge state $q_{m_i}^o$ ($i = 1$ to 4) for ion beams on heavy targets ($Z_2 \geq 12$) to find closer agreement with experiments.

Z_1	Z_2	E (MeV/u)	Final q_m^o
$4 \leq Z_1 \leq 10$	$12 \leq Z_2 \leq 39$	$0 < E \leq 4$	$q_{m_1}^o$
$4 \leq Z_1 \leq 10$	$40 \leq Z_2 \leq 54$	$E > 1.4$	$q_{m_1}^o + 0.8 Z_1/Z_2$
$4 \leq Z_1 \leq 10$	$54 < Z_2 \leq 92$	$E > 1.4$	$q_{m_1}^o + 1.5 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$12 \leq Z_2 \leq 18$	$0 < E \leq 1$	$q_{m_2}^o + 0.2 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$19 \leq Z_2 \leq 69$	$0 < E \leq 1$	$q_{m_2}^o + 0.7 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$70 \leq Z_2 \leq 92$	$0 < E \leq 1$	$q_{m_2}^o - 1.4 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$12 \leq Z_2 \leq 18$	$1 < E \leq 1.5$	$q_{m_2}^o + 0.05 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$19 \leq Z_2 \leq 46$	$1 < E \leq 1.5$	$q_{m_2}^o + 0.2 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$47 \leq Z_2 \leq 69$	$1 < E \leq 1.5$	$q_{m_2}^o + 1.2 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$70 \leq Z_2 \leq 92$	$1 < E \leq 1.5$	$q_{m_2}^o - 0.1 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$12 \leq Z_2 \leq 18$	$1.5 < E < 3.11$	$q_{m_2}^o - 0.05 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$19 \leq Z_2 \leq 47$	$1.5 < E \leq 3.11$	$q_{m_2}^o - 0.2 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$48 \leq Z_2 \leq 69$	$1.5 < E \leq 3.11$	$q_{m_2}^o + 1.2 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$70 \leq Z_2 \leq 92$	$1.5 < E \leq 3.11$	$q_{m_2}^o - 1.2 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$12 \leq Z_2 \leq 31$	$3.11 \leq E \leq 4$	$q_{m_2}^o - 0.3 Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$32 \leq Z_2 \leq 70$	$3.11 < E \leq 4$	$q_{m_2}^o - Z_1/Z_2$
$11 \leq Z_1 \leq 18$	$70 < Z_2 \leq 92$	$3.11 < E \leq 4$	$q_{m_2}^o - 2 Z_1/Z_2$
$19 \leq Z_1 \leq 54$	$12 \leq Z_2 \leq 27$	$0 \leq E \leq 4$	$q_{m_3}^o - 0.1 Z_1/Z_2$
$19 \leq Z_1 \leq 54$	$28 \leq Z_2 \leq 69$	$0 \leq E \leq 4$	$q_{m_3}^o - 0.4 Z_1/Z_2$
$19 \leq Z_1 \leq 54$	$70 \leq Z_2 \leq 92$	$0 \leq E \leq 4$	$q_{m_3}^o - Z_1/Z_2$
$55 \leq Z_1 \leq 92$	$12 \leq Z_2 \leq 47$	$0 \leq E \leq 4$	$q_{m_4}^o + 1.5 Z_2/Z_1$
$55 \leq Z_1 \leq 92$	$48 \leq Z_2 \leq 69$	$0 \leq E \leq 4$	$q_{m_4}^o + 1.2 Z_2/Z_1$
$55 \leq Z_1 \leq 92$	$70 \leq Z_2 \leq 92$	$0 \leq E \leq 4$	$q_{m_4}^o - 0.5 Z_2/Z_1$

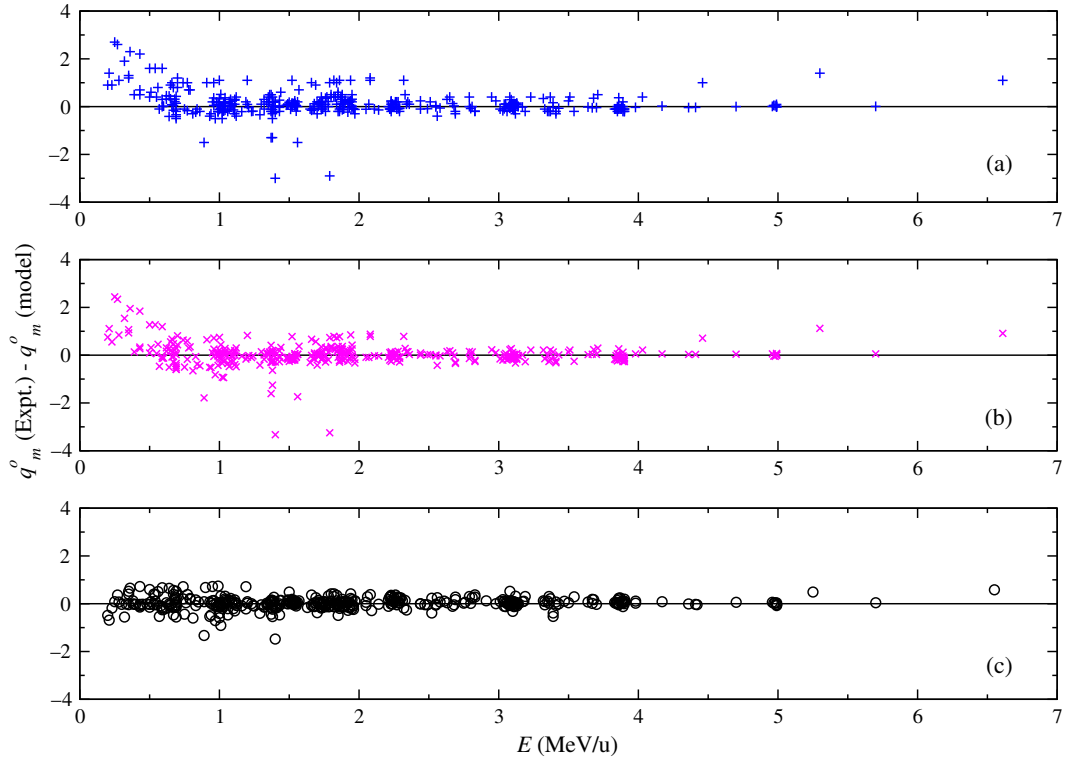


FIG. 9. Deviation of mean charge-state predictions of different models from the corresponding experimental mean charge states for different ion beams at different energies on different target foils: (a) q_m^o (Expt.) $- q_m^o$ (SGM), (b) q_m^o (Expt.) $- q_m^o$ (ISGM), and (c) q_m^o (Expt.) $- q_m^o$ (present).

two representative cases (a) and (b), i.e., for C and Si. RSSE is found as 0.0046, 0.0023, and 0.0017 for SGM, ISGM, and the present formula for calculating q_m^o . RSSE clearly indicated the usefulness of our proposed formulation for calculating q_m^o even in the case of light-ion beams. However, the scenario with other than carbon targets as shown in Fig. 8 with a solid line is not that good. To make it better, we have modified the Eqs. (17)–(20) by adding certain correction terms as given in Table I. The comparison of the experimental data with such modified equations is shown with the dotted lines. A good agreement is observed between the experimental data and the present estimates for all the groups.

The deviation of each model prediction from the experimental mean charge states is shown in Fig. 9. We can clearly see from Fig. 9 that the scattering of data is the lowest in present model. Therefore, we proceed to calculate the distribution width (Γ) using the present q_m^o values rather than SGM [Eq. (1)] or ISGM [Eq. (4)] for all ion-solid collision processes.

In the second step, the distribution width (Γ) of the projectile ion beam is calculated with an Eq. (9) taken from Novikov and Teplova [20], which corresponds to energy loss that occurred during the ion-solid collision process.

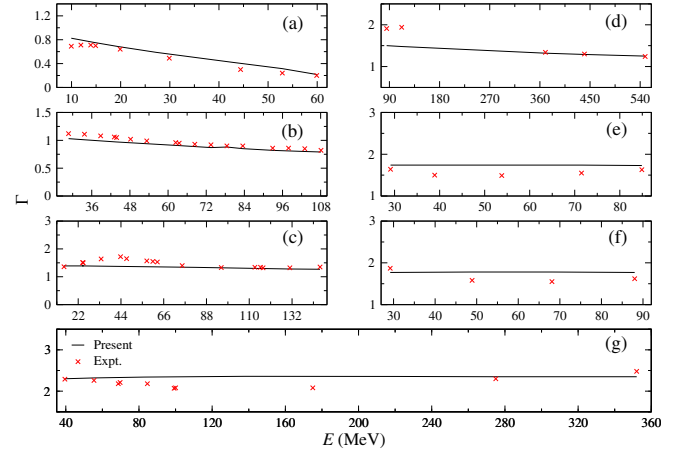


FIG. 10. Comparison of experimental charge-state distribution width (Γ) of different ion beams on carbon targets with theoretical values calculated by Eq. (9) as a function of beam energies. Experimental data for the projectile ions ^{12}C , ^{28}Si , ^{63}Cu , ^{83}Kr , and ^{197}Au are taken from Shima *et al.* [13]. While the data for ^{63}Cu , ^{107}Ag , ^{114}In and ^{197}Au ion beams are from Ball *et al.* [21]. Note that data for the projectiles ^{63}Cu and ^{197}Au are taken from both [13,21]. (a) C on C, (b) Si on C, (c) Cu on C, (d) Kr on C, (e) Ag on C, (f) In on C, and (g) Au on C.

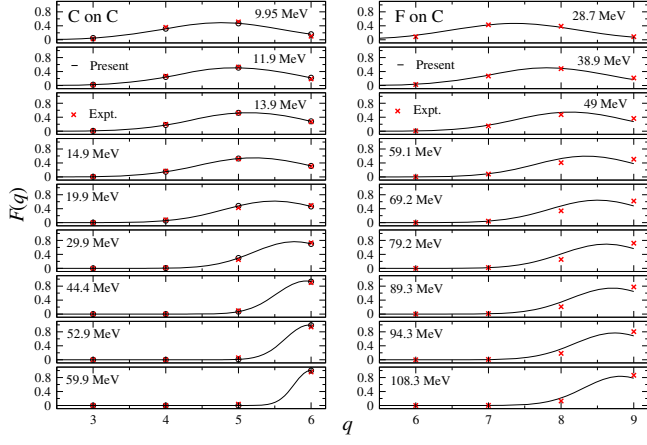


FIG. 11. Comparison of experimental charge-state distribution $[F(q) \text{ vs } q]$ for ^{12}C and ^{19}F ion beams at various beam energies [13] with our empirical Gaussian charge-state distribution where the distribution width Γ , charge-state fraction $F(q)$, and q_m^o are taken from Eqs. (9), (14), and (17), respectively.

Figure 10 represents the Γ values of ^{12}C , ^{28}Si , ^{63}Cu , ^{83}Kr , ^{107}Ag , ^{114}In , and ^{197}Au projectile ion beams for both theory and experimental values. Again, we can see a fair agreement between the theory and the experimental data which suggests that $\Gamma(x_1)$ [Eq. (9)] is a good choice for this theory. It may be noteworthy here that in some of the above figures—namely Figs. 1, 7, 9, and 10—either q_m^o or Γ was plotted as a function of emerging beam energy, which was estimated from the SRIM [22] code, unless stated otherwise in the corresponding reference.

In the third step, we have considered a Gaussian distribution from Shima *et al.* [13] and replaced its Γ with $\Gamma(x_1)$ [20] and use q_m^o from Eqs. (17)–(20) to obtain

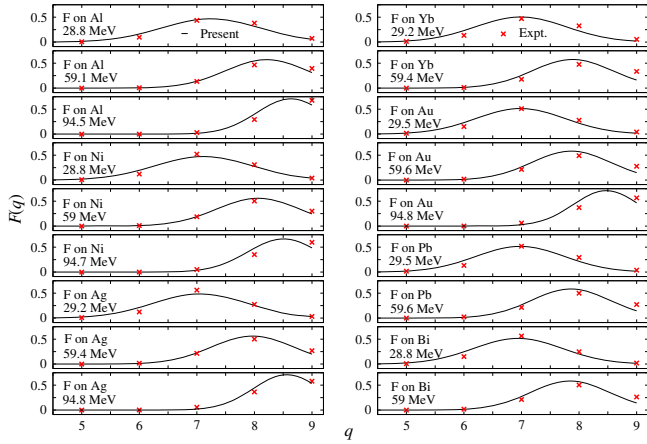


FIG. 12. Comparison of experimental charge-state distribution $[F(q) \text{ vs } q]$ for ^{19}F ion beams at various beam energies [13] with our empirical Gaussian charge-state distribution where the distribution width Γ , charge-state fraction $F(q)$, and q_m^o are taken from Eqs. (9), (14), and (17) along with corrections suggested in Table I, respectively.

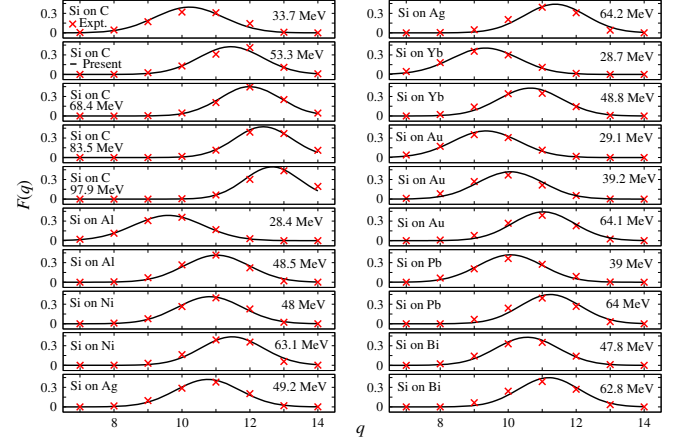


FIG. 13. Comparison of experimental charge-state distribution $[F(q) \text{ vs } q]$ for ^{28}Si ion beams at various beam energies [13] with our empirical Gaussian charge-state distribution where the distribution width Γ , charge-state fraction $F(q)$, and q_m^o are taken from Eqs. (9), (14), and (18) along with corrections suggested in Table I, respectively.

charge-state fraction values. An excellent agreement between theoretical and experimental CSD can be seen in Fig. 11, which represents the graphs of $F(q)$ versus q for the ^{12}C and ^{19}F projectile ion beams on the carbon target at various beam energies. The same scenarios can be observed in Fig. 12 for the ^{19}F projectile ion beam on light to heavy target foils, i.e., Al, Ni, Ag, Yb, Au, Pb, and Bi at different energies. It is very clear from Figs. 11 and 12 that the value of $F(q)$ is the highest at a certain value of q . This implies that q_m^o is quite close to this particular q . As the projectile ion beam increases, the mean charge state of the projectile

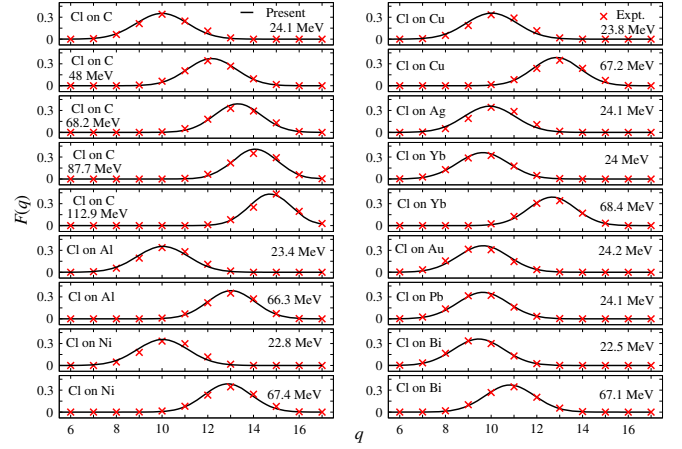


FIG. 14. Comparison of experimental charge-state distribution $[F(q) \text{ vs } q]$ for ^{35}Cl ion beams at various beam energies [13] with our empirical Gaussian charge-state distribution where the distribution width Γ , charge-state fraction $F(q)$, and q_m^o are taken from Eqs. (9), (14), and (18) along with corrections suggested in Table I, respectively.

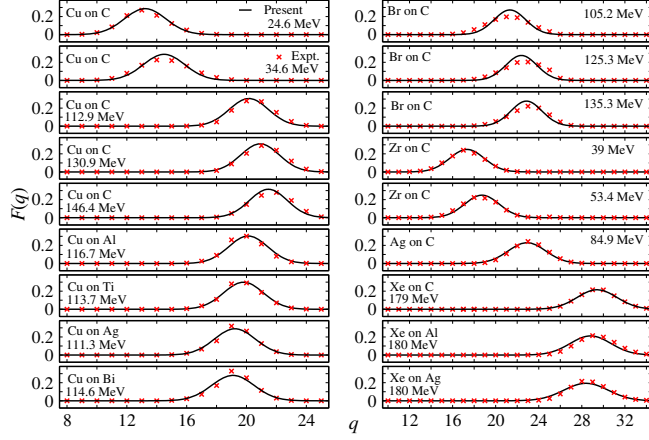


FIG. 15. Comparison of experimental charge-state distribution [$F(q)$ vs q] for ^{63}Cu , ^{80}Br , ^{91}Zr , ^{107}Ag , and ^{131}Xe ion beams at various beam energies [13,21] with our empirical Gaussian charge-state distribution where the distribution width Γ , charge-state fraction $F(q)$, and q_m^o are taken from Eqs. (9), (14), and (19) along with corrections suggested in Table I, respectively. The experimental $F(q)$ values for Cu ions at energies 24.6 and 34.6 MeV, and for Ag ions at energy 84.9 MeV are taken from Ball *et al.* [21], while rest of the cases are taken from Shima *et al.* [13].

ion shifts toward higher q values, which are much different from the incident charge state of the projectile ion beam.

A similar observation can be seen for the ions in group II. For example, the cases of projectile ion beams ^{28}Si and ^{35}Cl are shown for different target foils at different energies in Figs. 13 and 14, respectively. Here, in both Figs. 13 and 14,

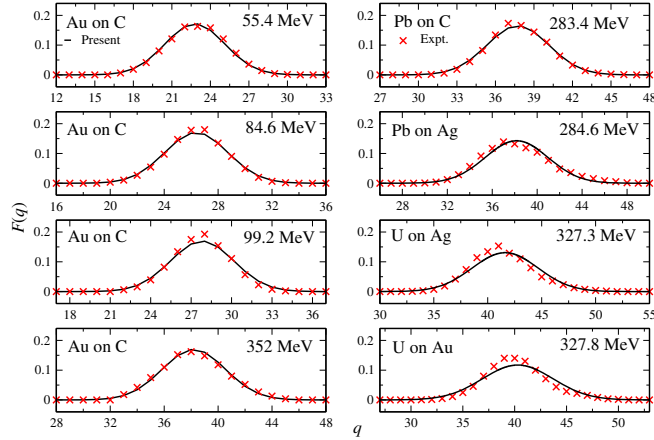


FIG. 16. Comparison of experimental charge-state distribution [$F(q)$ vs q] for ^{197}Au , ^{207}Pb and ^{238}U ion beams at various beam energies [13,21] with our empirical Gaussian charge-state distribution where the distribution width Γ , charge-state fraction $F(q)$, and q_m^o are taken from Eqs. (9), (14), and (20) along with corrections suggested in Table I, respectively. The experimental CSD values for Au ions at energies 55.4 and 84.6 MeV are taken from Ball *et al.* [21], while rest of the cases are taken from Shima *et al.* [13].

excellent agreement is observed between the present model and the experimental data. This implies that both q_m^o and $\Gamma(x_1)$ are predicted well by the present model.

Now comes the heavier projectile ion beams lying in group III. We have shown the CSD of ^{63}Cu , ^{80}Br , ^{91}Zr , ^{107}Ag , and ^{131}Xe on different target foils at different energies in Fig. 15. Here also, our predictions for CSD agree very well, as shown for the cases of ^{19}F , ^{28}Si , and ^{35}Cl .

Now, we proceed further toward much heavier projectile-ion beams lying in group IV. We see that the CSD for the heavy ions of ^{207}Pb and ^{238}U on the Ag and Au target foils, as shown in Fig. 16, gives an excellent match to the present predictions.

From the above comparisons, it is confirmed that the choice of the correction factors introduced to account for the variation of the values q_m^o with a heavier target is quite good. However, incorporating so many corrections is quite difficult for practical applications. To circumvent such inconveniences, we plan to develop a code that will be reported in an appropriate journal shortly.

VII. VALIDATION OF THE PRESENT MODEL

At a later stage, we searched again to find any further papers that can extend the experimental database. We found one on sulfur ions on the carbon target at 2 MeV/u [23]. We used the data reported here to validate our model. The present model considers experimental data obtained under equilibrium foil thickness conditions. We notice that this experiment has used various equilibrium foil thicknesses and also different charge states of the projectile ions. We picked up a case of S^{7+} projectile ions on three different foil thicknesses and another case of S^{12+} projectile ions on two different foil thicknesses. Different foil thicknesses will result in different energy losses in the foil, and slightly different results are therefore expected. The charge-state variation will hardly show any difference. Figure 17 shows exactly the same scenarios, and the agreement on the CSD between the experiment and the model prediction is pretty good. In addition, to check the agreement between the

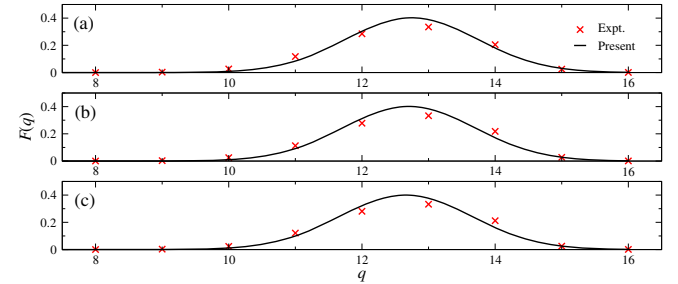


FIG. 17. Charge-state fraction $F(q)$ versus charge state q plot for 64 MeV S^{7+} ions on different carbon foil thicknesses. Foil thickness (t) and exit beam energy (E_{ex}) in figure are as follows: (a) $t = 54 \mu\text{g}/\text{cm}^2$ ($E_{\text{ex}} = 62.9 \text{ MeV}$), (b) $t = 98 \mu\text{g}/\text{cm}^2$ ($E_{\text{ex}} = 62 \text{ MeV}$), and (c) $t = 150 \mu\text{g}/\text{cm}^2$ ($E_{\text{ex}} = 61 \text{ MeV}$).

TABLE II. Comparison of charge-state fraction $[F(q)]$, mean charge state (q_m^o), and distribution width (Γ) between predictions of the present model (our) and experimental data [23] (Expt.). Note that charge state of the incident ions is denoted by q_{in} and foil thickness by t in $\mu\text{g}/\text{cm}^2$.

q_{in}	t	Charge-state fraction												q_m^o	Γ
		S^{7+}	S^{6+}	S^{7+}	S^{8+}	S^{9+}	S^{10+}	S^{11+}	S^{12+}	S^{13+}	S^{14+}	S^{15+}	S^{16+}		
Expt. S^{7+}	54	1.26×10^{-7}		6.71×10^{-6}	1.91×10^{-4}	3.03×10^{-3}	2.64×10^{-2}	1.18×10^{-1}	2.85×10^{-1}	3.35×10^{-1}	2.05×10^{-1}	2.53×10^{-2}	1.13×10^{-3}	12.64	1.113
Our		3.62×10^{-11}		2.07×10^{-8}	4.28×10^{-5}	3.20×10^{-4}	8.69×10^{-3}	8.53×10^{-2}	3.03×10^{-1}	3.89×10^{-1}	1.81×10^{-1}	3.05×10^{-2}	1.86×10^{-3}	12.74	0.991
Expt. S^{7+}	98	1.51×10^{-7}		7.20×10^{-6}	2.00×10^{-4}	2.87×10^{-3}	2.52×10^{-2}	1.13×10^{-1}	2.78×10^{-1}	3.33×10^{-1}	2.18×10^{-1}	2.75×10^{-2}	1.34×10^{-3}	12.68	1.118
Our		5.40×10^{-11}		2.86×10^{-8}	5.53×10^{-6}	3.88×10^{-4}	9.92×10^{-3}	9.22×10^{-2}	3.12×10^{-1}	3.84×10^{-1}	1.72×10^{-1}	2.80×10^{-2}	1.66×10^{-3}	12.70	0.994
Expt. S^{7+}	150	...		6.73×10^{-6}	1.77×10^{-4}	2.72×10^{-3}	2.34×10^{-2}	1.21×10^{-1}	2.81×10^{-1}	3.33×10^{-1}	2.12×10^{-1}	2.49×10^{-2}	1.18×10^{-3}	12.66	1.109
Our				4.11×10^{-8}	7.35×10^{-6}	4.80×10^{-4}	1.15×10^{-2}	1.00×10^{-1}	3.22×10^{-1}	3.77×10^{-1}	1.62×10^{-1}	2.53×10^{-2}	1.45×10^{-3}	12.65	0.997
Expt. S^{12+}	54	1.60×10^{-7}		6.87×10^{-6}	1.90×10^{-4}	3.00×10^{-3}	2.60×10^{-2}	1.25×10^{-1}	2.82×10^{-1}	3.49×10^{-1}	1.89×10^{-1}	2.41×10^{-2}	1.04×10^{-3}	12.62	1.104
Our		3.62×10^{-11}		2.07×10^{-8}	4.28×10^{-5}	3.20×10^{-4}	8.69×10^{-3}	8.53×10^{-2}	3.03×10^{-1}	3.89×10^{-1}	1.81×10^{-1}	3.05×10^{-2}	1.86×10^{-3}	12.74	0.991
Expt. S^{12+}	98	...		6.45×10^{-6}	1.75×10^{-4}	2.68×10^{-3}	2.41×10^{-2}	1.13×10^{-1}	2.78×10^{-1}	3.43×10^{-1}	2.11×10^{-1}	2.67×10^{-2}	1.23×10^{-3}	12.68	1.105
Our		5.40×10^{-11}		2.86×10^{-8}	5.53×10^{-6}	3.88×10^{-4}	9.92×10^{-3}	9.22×10^{-2}	3.12×10^{-1}	3.84×10^{-1}	1.72×10^{-1}	2.80×10^{-2}	1.66×10^{-3}	12.70	0.994
Expt. S^{14+}	54	1.83×10^{-7}		6.98×10^{-6}	1.99×10^{-4}	3.01×10^{-3}	2.64×10^{-2}	1.20×10^{-1}	2.90×10^{-1}	3.34×10^{-1}	2.01×10^{-1}	2.51×10^{-2}	1.09×10^{-3}	12.63	1.112
Our		3.62×10^{-11}		2.07×10^{-8}	4.28×10^{-5}	3.20×10^{-4}	8.69×10^{-3}	8.53×10^{-2}	3.03×10^{-1}	3.89×10^{-1}	1.81×10^{-1}	3.05×10^{-2}	1.86×10^{-3}	12.74	0.991
Expt. S^{16+}	98	...		4.56×10^{-6}	1.39×10^{-4}	2.22×10^{-3}	2.01×10^{-2}	9.64×10^{-2}	2.49×10^{-1}	3.38×10^{-1}	2.55×10^{-1}	3.76×10^{-2}	1.95×10^{-3}	12.82	1.116
Our		5.40×10^{-11}		2.86×10^{-8}	5.53×10^{-6}	3.88×10^{-4}	9.92×10^{-3}	9.22×10^{-2}	3.12×10^{-1}	3.84×10^{-1}	1.72×10^{-1}	2.80×10^{-2}	1.66×10^{-3}	12.70	0.994
Expt. S^{16+}	150	...		4.05×10^{-6}	1.51×10^{-4}	2.80×10^{-3}	3.10×10^{-2}	1.24×10^{-1}	2.91×10^{-1}	3.22×10^{-1}	2.05×10^{-1}	2.41×10^{-2}	1.02×10^{-3}	12.61	1.129
Our				4.11×10^{-8}	7.35×10^{-6}	4.80×10^{-4}	1.148×10^{-2}	1.00×10^{-1}	3.22×10^{-1}	3.77×10^{-1}	1.62×10^{-1}	2.53×10^{-2}	1.45×10^{-3}	12.65	0.997
Expt. S^{16+}	200	...		8.07×10^{-6}	2.01×10^{-4}	3.31×10^{-3}	2.89×10^{-2}	1.29×10^{-1}	3.00×10^{-1}	3.27×10^{-1}	1.89×10^{-1}	2.09×10^{-2}	8.72×10^{-4}	12.57	1.112
Our				4.26×10^{-8}	7.55×10^{-6}	4.90×10^{-4}	1.16×10^{-2}	1.01×10^{-1}	3.22×10^{-1}	3.76×10^{-1}	1.60×10^{-1}	2.50×10^{-2}	1.43×10^{-3}	12.65	0.997

measured $F(q)$, q_m^o and Γ with the predictions of the present model, we compared our predictions with the full dataset given by Imai *et al.* [23] in Table II. An excellent match found for all the quantities justifies the worth of the present model.

VIII. CONCLUSION

The charge-state distributions (CSD) of projectile ions through gaseous or solid targets in the energy range of tandem accelerators ($1 \text{ MeV/u} < E < 4 \text{ MeV/u}$) have a major impact on ion-atom collisions and accelerator physics. Theoretically, it is possible to calculate the CSD for up to Ni-like ions, but empirical models do not have such bounds. In recent decades, the mean charge states (q_m^o) have been obtained primarily from an empirical formula [9]. However, no description of CSD is found there. To estimate the CSD, we have used a Gaussian distribution function having distribution width given by Novikov and Teplova [20]. The results obtained are compared with those obtained with the measured CSD for heavy projectile ions. We notice that it works well, but its validity range is restricted by the correct values of q_m^o , which are limited only to the projectile atomic number $Z_1 \leq 16$. Empirically, q_m^o is estimated in terms of a reduced parameter x_{01} [Eq. (2)] or x_{02} [Eq. (5)]. Instead of using x_{02} , we use x_{01} and develop a new model, which classifies the full range of projectiles into four groups to estimate q_m^o in good agreement with the experimental counterparts with the carbon targets. However, using this model to find q_m^o for heavier targets shows a certain deviation from the experimental counterparts. To minimize this difference, we added certain correction terms with the formulas for q_m^o . The q_m^o so obtained shows good agreement with the experimental scenarios. Using such q_m^o , we proceed to calculate the CSD in the above-mentioned way. The CSDs so obtained are found to be very close to the experimental values [13,21]. Finally, excellent agreement between our predictions with a different set of experimental data [23] validates the worth of the present model.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The data that support the findings of this article are openly available [11,13,21], embargo periods may apply.

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