Born cross sections for fast, low-charge-state uranium ions colliding with lithium atoms and ions

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Born-approximation calculations of various inelastic-scattering cross sections for collisions between U^{q+} ($q = 1$, 2, and 4) ions and Li atoms and ions are presented. The energies considered are in the 10–100-MeV/amu regime, with an emphasis on providing results useful in assessing the importance of various phenomena in heavy-ion, inertial-confinement-fusion reactor concepts for the case of U^{1+} beams of 10–20 GeV. Estimates of the U^{q+} electron-loss cross sections are given for collisions with lithium in all charge states; order-of-magnitude differences between Li atoms and ions are predicted. Calculations of the cross sections for the ionization of Li atoms and ions due to the impact of fast U^{q+} ions are also given. The lithium discrete-state and ionization contributions to the sum-rule asymptotic cross sections are computed for the cases of Li^0 and Li^{2+}. Ionization is the dominate contributor ($> 50\%$) for these collisions, in contrast to the case of proton impact at similar speeds ($\lesssim 10\%$ for Li^0). We also estimate the mean energies of the electrons produced in these ionizing collisions and obtain results more than an order of magnitude larger than in the case of proton impact.

I. INTRODUCTION

The use of intense beams of high-energy heavy ions for the compression and ignition of small pellets containing thermonuclear fuel has received considerable attention in recent years as an attractive future option for energy production.[1-4] As an inertial confinement fusion (ICF) driver competitive with lasers, and with electron and light-ion beams, heavy ions offer potential advantages in terms of driver efficiency, pellet coupling, and a substantial technological base of high-energy accelerators. As a relatively new approach to fusion, there are a number of scientific and technical questions which must still be addressed.

One area of concern has been the potential difficulties associated with the propagation of heavy-ion beams to a small pellet in the environment of an ICF reactor.[5-8] Beam propagation in a moderate vacuum (10^{-3}–10^{-4} Torr) has been identified[7,8] as a baseline transport scenario which merits increased attention. Because the physics of the beam propagation is relatively simple in this case, theoretical predictions of the characteristics of this propagation mode can be made with reasonable confidence. Perhaps more importantly, this scenario is also consistent with various ICF reactor concepts such as the HYLIFE design which utilizes liquid lithium jets for first wall protection.[9] A critical parameter in the design of such reactors, or advanced versions which utilize lead-lithium compositions, is the allowable operating pressure.[10] This is generally determined by the degree of permissible electron stripping from the beam ions in collisions with the gases present in the reactor, since, depending on other parameters of the beam and reactor, beam ions whose charge state is changed are effectively removed from that part of the beam which hits the target.[11] This paper presents the results of a theoretical investigation of high-energy inelastic collision processes for fast uranium ions impacting on lithium atoms and ions, with an emphasis on beam electron stripping and target gas ionization. We also present the methodology and results of calculations for the mean kinetic energy of electrons produced in impact ionization of lithium by fast uranium ions. In a separate paper,[11] our results are applied to the study of heavy-ion beam propagation in the environment of a liquid lithium ICF reactor.

II. BORN-APPROXIMATION CROSS-SECTION CALCULATIONS

A. U^{q+} electron-stripping cross section

The basic theory underlying the calculations of this work has been described previously[12] and only the results required for this problem will be given. A number of refinements have also been examined in an effort to provide a better assessment of the reliability of the computed cross sections, since the charge state and energy regime for these collisions is significantly beyond that where experimental data are available. The starting point for these calculations is the momentum-transfer formulation of the Born approximation for inelastic cross sections. For the ionization of a fast ion colliding with a neutral atom (i.e., electron stripping) the cross section consists of two contributions, corresponding to whether the target atom is scattered elastically (el) or inelastically (in). Following the notation of Ref. 12, the stripping cross section for a U^{q+} ion may be written as

$$\sigma_{\text{stripping}} = \sigma(\text{U}^{q+})_{\text{ion}} = \sigma_{\text{ion, el}} + \sigma_{\text{ion, in}} \ , \tag{1}$$

where in Born approximation at high energies

$$\sigma_{\text{ion, el}} = 8\pi a_0^2 \frac{\alpha^2}{\beta^2}\left(I_{\text{ion, el}} + \gamma_{\text{ion, el}}\frac{\alpha^2}{\beta^2} + \cdots\right) , \tag{2}$$

$$\sigma_{\text{ion, in}} = 8\pi a_0^2 \frac{\alpha^2}{\beta^2}\left(I_{\text{ion, in}} + \gamma_{\text{ion, in}}\frac{\alpha^2}{\beta^2} + \cdots\right) . \tag{3}$$

The terms in parentheses in Eqs. (2) and (3) are the collision strengths as calculated to two orders in an expansion in inverse powers of the ion velocity v ($\beta = v/c$). Calculation of the coefficients of these terms requires detailed information on the continuum transition strengths, or equivalently the generalized oscillator strengths, for the U^{q+} ion. Such information for low-charge-state heavy ions is generally not available, and the calculation of such data can be a major undertaking in itself.[13] An upper bound to these coefficients can be established by calculating (via closure) the collision strengths for all inelastic final states of the incident ion. Equations (2) and (3) are thus replaced by Eqs. (2) and (3) of Ref. 12, and Eq. (1) becomes an inequality, viz.,

$$\sigma(\text{U}^{q+})_{\text{ion}} \leq \sigma_{\text{in, el}} + \sigma_{\text{in, in}} \ , \tag{4}$$

where

$$\sigma_{\text{in, el}} = 8\pi a_0^2 \frac{\alpha^2}{\beta^2}\left(I_{\text{in, el}} + \gamma_{\text{in, el}}\frac{\alpha^2}{\beta^2}\right), \tag{5}$$

$$\sigma_{\text{in, in}} = 8\pi a_0^2 \frac{\alpha^2}{\beta^2}\left(I_{\text{in, in}} + \gamma_{\text{in, in}}\frac{\alpha^2}{\beta^2}\right). \tag{6}$$

The collision strength parameters ($I_{\text{in, el}}$, $\gamma_{\text{in, el}}$, $I_{\text{in, in}}$, and $\gamma_{\text{in, in}}$) only require ground-state properties of the U^{q+} ion and the target atom.[12]

If the background Li gas is partially ionized, then the effective stripping cross sections can change significantly. Since ionized target particles have a long-range term in the potential for interaction with the projectiles' electrons, the asymptotic form of the stripping cross sections is altered. Again using closure, it is possible to provide upper bounds to the stripping cross section via Eq. (4), where Eq. (5) assumes the form

$$\sigma_{\text{in, el}} = 4\pi a_0^2 \frac{\alpha^2}{\beta^2}\left(|F_0^{(2)}(0)|^2 S^{(1)}(-1)(\ln\beta^2\gamma^2 - \beta^2) + C_{\text{in, el}} + 2\gamma_{\text{in, el}}\frac{\alpha^2}{\beta^2}\right). \tag{7}$$

The form of Eq. (6) is unchanged, although the numerical values of the collision strength parameters $I_{\text{in, in}}$ and $\gamma_{\text{in, in}}$ will be different.

In Eq. (7), $F_0^{(2)}(0)$ is the net charge of the ionized Li target (i.e., 1, 2, or 3), $S^{(1)}(-1)$ is the -1 energy moment of the uranium ion dipole-oscillator-strength distribution, and $\gamma^2 = (1-\beta^2)^{-1}$. $C_{\text{in, el}}$ is a collision strength parameter which may be calculated analogously to that described in Ref. 12 (noting that here one is considering the inelastic scattering of the projectile by a charged target ion). It depends (via sum rules) on the ground-state properties of both the incident uranium ion and the target lithium ion, as well as on one property of the uranium ion which cannot be calculated directly from the ground state: the -1 logarithmic energy moment of dipole-oscillator-strength distribution $L(-1)$. A method for estimating this parameter is described later in this section.

Calculation of the asymptotic collision strengths ($I_{\text{in, el}}$ and $I_{\text{in, in}}$) for several charge states of U^{q+} colliding with neutral lithium were reported previously.[14] Relativistic Hartree-Fock wave functions were used to obtain the U^{q+} ion incoherent scattering functions, which are required to evaluate $I_{\text{in, el}}$ and $I_{\text{in,in}}$ in Eqs. (5) and (6) as well as $C_{\text{in, el}}$ in Eq. (7). These same functions[15] have been utilized in the calculations reported here. Hartree-Fock wave functions were used in the previous report[14] for the elastic form factor and incoherent scattering function for neutral lithium. In this paper, calculations have utilized results for these functions tabulated by Hubbell *et al.*,[16] which are based on neutral Li wave functions calculated by Brown[17] and include configuration interactions. For Li^+, calculations have been carried out using data based on two different ground-state wave functions. One is a simple $1s^2$ hydrogenic wave function with an effective $Z = 2 + \frac{11}{16}$; the other is a 53-term Weiss wave function for which the atomic form factor and incoherent scattering functions have been given by Kim.[18] For Li^{2+} the analytic forms for these functions have been used.[19]

In order to calculate the second-order collision strengths ($\gamma_{\text{in, el}}$ and $\gamma_{\text{in, in}}$) in Eqs. (5) and (6), as well as the parameters in Eq. (7) for collisions with ionized lithium, a number of additional atomic constants for uranium ions and lithium atoms and ions are needed. In Table I some results of a survey of the available data[19-26] for various charge states of lithium are summarized. Table II provides a summary of select data for several heavy atoms and low-charge-state heavy ions, together with some estimated data for U^{q+} ions.[12,15,16,28-32] The notation corresponds to that in Ref. 12, and not all these parameters will be discussed here. Only a few comments regarding some of the estimated parameters are presented.

Various energy moments of the oscillator-strength distribution are required in order to

TABLE I. Summary of select oscillator-strength data for Li atoms and ions. The $S(\mu)$ ($\mu=-1,0,+1$) are the μth energy moments of the dipole-oscillator-strength distributions, and $L(-1)$ is the -1 logarithmic energy moment of that distribution. $S'(1)$ is the first derivative with respect to K^2 of the $+1$ energy moment of the generalized-oscillator-strength distribution. Parameters labeled by the subscript "ion" are the contributions to these moments arising from final states in the continuum (including inner-shell excitation for Li^0) which lead to ionization.

Atom / Ion	$S(-1)$	$S(0)$	$S(1)$	$L(-1)$	$S'(1)$	$S(-1)_{ion}$	$S(0)_{ion}$	$S(1)_{ion}$	$L(-1)_{ion}$	$S'(1)_{ion}$	$F_0'(0)$
Li^0	6.037 [a]	3	20.74 [a]								3.062 [a]
	5.865 [b]	3	21.0 [b]	−9.92 [b]		0.495 [c]	2.22 [c]		0.492 [c]		
	6.189 [d]	3	19.82 [d]		3.08	0.489 [e]	2.22 [e]	19.71 [d]		2.48 [e]	3.105
Li^+	0.2860 [f]	2	20.18 [f]	0.5277 [f]	2.024 [f]	0.1445 [f]	1.324 [f]	16.94 [f]	0.3068 [f]	3.104 [f]	0.1488
Li^{2+}	$\frac{1}{9}$ [g]	1	12 [g]	0.2360 [h]	1.0000	0.03149 [g]	0.4350 [g]	7.956 [g]	0.08029 [h]	1.6476	$\frac{1}{18}$

[a]Based on configuration-interaction wave functions: $S(-1)$, Ref. 21; $S(+1)$ and $F_0'(0)$, Ref. 20.
[b]Based on Herman-Skillman model, Ref. 21.
[c]Based on Herman-Skillman model, Ref. 22.
[d]Hartree-Fock values, Ref. 23.
[e]Hartree-Fock values, Ref. 24.
[f]Reference 25.
[g]Reference 19.
[h]Calculated according to Eq. (13) using hydrogen data, Ref. 26.

evaluate $\gamma_{in,el}$ and $\gamma_{in,in}$. Most of these can be calculated from ground-state wave functions using well-known sum rules.[12] For the uranium ions under consideration, the -1 energy moment $S(-1)$ has been calculated[15] and the zeroth moment $S(0)$ is simply equal to the number of electrons. The energy moment $S(1)$ has not been calculated directly, but is closely related to the total

TABLE II. Summary of select atomic data for heavy atoms and ions and values adopted for U^{q+}. The $S(\mu)$ ($\mu=-1,0,+1$) are the μth energy moments of the dipole-oscillator-strength distributions, and $L(-1)$ is the -1 logarithmic energy moment of that distribution as calculated according to Eq. (12). Also given are the total energies E_{tot}, which are used with Eq. (8) and some known values for $S(1)$ to calculate $\Omega_p/\Sigma p^2$. The results for neutral atoms, and for Cs^+ and Au^+, are used to estimate the value of -0.39 ± 0.03 for U^{q+} which then allows an estimate of $S(1)$ for these ions according to Eq. (8). [In addition to E_{tot} and $\Omega_p/\Sigma p^2$, the ionization contribution to the -1 energy moment $S(-1)_{ion}$ and the ionization potential E_B are also included where known, although they are not directly used in the cross-section computations.]

Atom \ Ion	$S(-1)$	$S(0)$	$S(1)$	$L(-1)$	E_{tot} (Ry)	$\Omega_p/\Sigma p^2$	$S(-1)_{ion}$	$F_0'(0)$	E_B(Ry)
Kr	7.864 [a]	36	5.340×10^3 [a]	6.1	5.504×10^3 [b]	−0.272	6.09 ± 0.16 [c]	6.588 [b]	1.029 [d]
Xe	11.78 [a]	54	1.313×10^4 [a]	7.9	1.446×10^4 [b]	−0.319	8.04 ± 0.15 [c]	10.44 [b]	0.892 [d]
Hg	15.6 [e]	80			3.682×10^4 [b]		5.69 ± 0.94 [c]	11.44 [b]	0.790 [d]
Rn	14.57 [a]	86	3.634×10^4 [a]	13	4.373×10^4 [b]	−0.377		13.54 [b]	0.790 [d]
Xe^+	9.554 [f]	53					~1.3 ± 0.7 [g]	8.52 [f]	1.56 [d]
Cs^+	9.417 [h]	54	1.37×10^4 [h]	8.8	1.511×10^4 [i]	−0.320		8.537 [h]	1.85 [d]
Au^+	9.166 [h]	78	3.01×10^4 [h]	12	3.573×10^4 [i]	−0.368		7.914 [h]	1.51 [d]
U^+	19.78 [f]	91	$4.6(\pm0.2)\times10^4$	10 ± 5	5.603×10^4 [f]	−0.39 ± 0.03		14.43 [f]	0.855 [j]
U^{2+}	16.25 [f]	90	$4.6(\pm0.2)\times10^4$	12 ± 6	5.603×10^4 [f]	−0.39 ± 0.03		12.49 [f]	1.33 [j]
U^{4+}	12.29 [f]	88	$4.6(\pm0.2)\times10^4$	13 ± 6	5.602×10^4 [f]	−0.39 ± 0.03		10.09 [f]	3.67 [j]

[a]Hartree-Fock values from Ref. 28.
[b]Hartree-Fock values from Ref. 29.
[c]Experimental data for fast electrons, Ref. 30.
[d]Reference 31.
[e]Estimated from low-K behavior of incoherent scattering function tabulated in Ref. 16.
[f]Dirac-Hartree-Fock values from Ref. 15.
[g]Estimated from experimental data on electron impact ionization, Ref. 32.
[h]Reference 12.
[i]Hartree-Fock values from Ref. 33.
[j]Reference 34.

energy $E_{\rm tot}$ of the ion. In particular

$$S(1)=\tfrac{4}{3}E_{\rm tot}(1+\Omega_p/\Sigma p^2)\ , \tag{8}$$

where $E_{\rm tot}$ is in Rydbergs and

$$\Omega_p/\Sigma p^2=\sum_{j,k\neq j}\langle\vec{P}_j\cdot\vec{P}_k\rangle\sum_j\langle\vec{P}_j^2\rangle\ . \tag{9}$$

The $\langle\ \rangle$ denotes ground-state expectation values and the sums are over electrons. This term gives a measure of the relative importance of electron correlations to the +1 energy moment.[27] It is generally a slowly varying function of the atomic number; for example, it varies between +0.05 and −0.10 for the atoms He-Ne, and approaches −0.4 for heavy atoms. In order to estimate values of $S(1)$ for U^{q+} ions, values of $\Omega_p/\Sigma p^2$ were calculated for several heavy atoms and ions for which $E_{\rm tot}$ and $S(1)$ are known. The results are given in Table II. From this data an extrapolation to uranium ions yielded the value −0.39 ± 0.03. Together with the relativistic Hartree-Fock values of the total energy for U^{q+} ions,[15] Eq. (8) could then be used to estimate $S(1)$ for these ions. The adopted values are those given in Table II, as calculated by this procedure. Within this approximation, the results for $S(1)$ for U^{1+}, U^{2+}, and U^{4+} are essentially the same.

As indicated previously, calculation of the parameter $C_{\rm in,el}$ appearing in Eq. (7), for estimating electron stripping from U^{q+} in collisions with ionized lithium, the −1 logarithmic energy moment of the U^{q+} dipole-oscillator-strength distribution is required. This constant is difficult to calculate in general because it requires detailed knowledge of that distribution; it cannot be simply related to a ground-state expectation value. If one has sufficient information on the energy moments $S(\mu)$, as a continuous function of μ, then it is possible to calculate $L(-1)$ since, in general,

$$L(\mu)=\frac{d}{d\mu}S(\mu)\ . \tag{10}$$

A simplified version of the analytic form of $S(\mu)$ suggested by Bell *et al.*[28] has been adopted. Specifically, $S(\mu)$ is assumed to be of the form

$$S(\mu)=S(0)\exp[\mu a+\mu b/(5-2\mu)]\ . \tag{11}$$

This form incorporates the known singularity at $\mu=\frac{5}{2}$ and behaves correctly as μ approaches $-\infty$. The constants a and b are determined so that Eq. (11) reproduces the moments $S(-1)$ and $S(1)$. $L(-1)$ can then be calculated according to Eq. (10); i.e.,

$$L(\mu)=S(\mu)[a+5b/(5-2\mu)^2]\ , \tag{12}$$

evaluated at $\mu=-1$. A number of similar models were examined, including some which incorporate additional moments such as $S(-2)$. However, they generally gave poor results for $L(-1)$, although they often yielded good values for $L(0)$ and $L(1)$ important in energy-loss and straggling computations. Equation (12) for $L(-1)$ was tested for the 18 elements from H to Ar by utilizing the Herman-Skillman model data of Dehmer *et al.*[21] for $S(-1)$, $S(0)$, and $S(1)$. The calculated values of $L(-1)$ ranged from −7.2 to 3.3, as compared to the range from −10 to +2.5 for the Herman-Skillman model.[21] Equation (12) always estimates a larger value of $L(-1)$ than the Herman-Skillman results, predicts the same sign in all but two cases [C and P, which have small, negative values of $L(-1)$], and is most reliable for positive values of $L(-1)$.

Table II gives results for $L(-1)$ calculated this way using the data for the $S(\mu)$ also given in the table. Among the atoms and ions considered, the only other results for this parameter known to us are a Hartree-Slater value of 3.75 for Kr, about 40% lower than our estimate, and moment theory results of 6.2 for Kr and 10 for Xe, about 2% and 27% above our estimates.[27] We have tentatively assigned a ±50% uncertainty to our estimates of $L(-1)$ for U^{q+}. However, as noted in previous work[12] the cross-section calculations do not depend strongly on this parameter, if its magnitude is small ($\lesssim 20$).

The various energy moments of the oscillator strength distribution for lithium atoms or ions given in Table I have been extracted from the literature, with the exception of the $L(-1)$ values for Li^{2+}. Since this is a hydrogenic ion, it is possible to scale this parameter from atomic hydrogen data. From the known Z dependence of the excitation energy and oscillator strengths[19] one can show that for hydrogenic ions

$$L^Z(\mu)=Z^{2\mu}[2S(\mu)\ln Z+L(\mu)]\ , \tag{13}$$

where $S(\mu)$ and $L(\mu)$ are the atomic hydrogen values for these moments. This formula is also valid for the contributions arising from continuum final states $L^Z(\mu)_{\rm ion}$, with $S(\mu)$ and $L(\mu)$ replaced by the corresponding contributions for hydrogen.[26]

Table III summarizes the results of the calculations for the collision strength parameters appearing in Eqs. (5)–(7), for U^{q+} ions ($q=1$, 2, and 4) colliding with all charge states of Li. We also have explicitly given the values of the momentum-transfer integral $\mathcal{I}_1-\mathcal{I}_2$, for impact with lithium ions, which are required to evaluate $C_{\rm in,el}$:

$$C_{\rm in,el}=|F_0^{(2)}(0)|^2[S^{(1)}(-1)\ln 4/\alpha^2-2L^{(1)}(-1)]+(\mathcal{I}_1-\mathcal{I}_2)\ . \tag{14}$$

TABLE III. Collision strength parameters for the inelastic scattering of U^{q+} ions ($q=1,2,4$) by lithium atoms and ions. For U^{+}, results are presented for different atomic models of neutral Li and Li^{+} as described more fully in the text. However, the results show little sensitivity to the different models. These results, together with $S^{(1)}(-1)$ for the uranium ions given in Table II and the net charge on the lithium ion [$F_0^{(2)}(0)=1$, 2, or 3] can be used with Eqs. (5)–(7) to calculate upper bounds on the U^{q+} electron-stripping cross sections according to Eq. (4).

Projectile	Target	$I_{\text{in, el}}$ (or $\mathcal{I}_1-\mathcal{I}_2$)	$I_{\text{in, in}}$	$C_{\text{in, el}}$	$\gamma_{\text{in, el}}$	$\gamma_{\text{in, in}}$
U^{1+}	Li^0 (HF)	29.5 [a]	32.6 [a]			
	Li^0 (CI)	29.4	32.1		-1.02×10^{2}	-3.49×10^{4}
	Li^+ ($1s^2$)	(30.4)	8.52			
	Li^+ (CI)	(30.5 ± 0.9)	8.51 ± 0.09	233 ± 11	-1.83×10^{3}	-1.76×10^{3}
	Li^{2+}	(11.5 ± 0.4)	3.77	820 ± 41	-1.43×10^{3}	-7.03×10^{2}
	Li^{3+}	9 × (−2.55 ± 0.08)	0	1790 ± 90	-2.05×10^{2}	0
U^{2+}	Li^0 (CI)	27.9	29.3		-1.01×10^{2}	-3.49×10^{4}
	Li^+ (CI)	(34.6 ± 1.3)	8.10 ± 0.1	193 ± 13	-1.82×10^{3}	-1.75×10^{3}
	Li^{2+}	(30.5)	3.59	664 ± 48	-1.42×10^{3}	-6.97×10^{2}
	Li^{3+}	9 × (2.40 ± 0.06)	0	1450 ± 110	-2.03×10^{2}	0
U^{4+}	Li^0 (CI)	25.5	25.4		−99.0	-3.48×10^{4}
	Li^+ (CI)	(36.3)	7.42	148 ± 13	-1.82×10^{3}	-1.74×10^{3}
	Li^{2+}	(44.8)	3.30	493 ± 48	-1.42×10^{3}	-6.90×10^{2}
	Li^{3+}	9 × (3.36)	0	1040 ± 110	-1.98×10^{2}	0

[a] From Ref. 14.

The cross sections for the inelastic scattering of U^+ colliding with different charge states of lithium are shown in Fig. 1 in the 10–100-MeV/amu energy regime. For comparison both the asymptotic cross section (leading order in β^{-2} expansion) and the cross section as calculated here to two orders in the inverse velocity expansion are shown by broken and solid curves, respectively. Significant corrections to the asymptotic cross section for collisions with neutral lithium targets are apparent for this energy range, whereas only minor deviations occur for ionized lithium targets. In these latter cases, the cross sections are also significantly larger in magnitude throughout this energy range. Figure 2 gives results for U^{2+} and U^{4+} ions, in these cases the cross sections plotted retain two orders in the expansion.

The cross sections in Figs. 1 and 2 should provide reliable upper bounds to the total electron-stripping cross sections for uranium ions. The generally slow variation of all the cross sections as a function of the uranium ion charge state suggest that U^{3+} cross sections can be readily estimated by interpolation. Extrapolation to modestly higher charge states ($q\leq 8$) can be accomplished with reasonable accuracy by scaling the U^{4+} cross sections according to the ratios for the cross sections for U^{q+} colliding with Li reported in Ref. 14. Note, however, that the overall magnitudes of the cross sections reported here are somewhat lower.

Two further questions arise regarding the utility of these inelastic cross sections for calculating electron-stripping data (as opposed to establishing upper-bound cross sections). One concerns the relative contributions of projectile excitation and ionization[19]; the other concerns the final charge-state distribution of the ions following electron stripping. For somewhat higher initial charge states, Dmitriev *et al.*[36] have recently reported results of semiempirical calculations of the cross sections for the loss of from 1 to 5 electrons for U^{q+} ($q\geq 10$) and I^{q+} ($q\geq 5$) ions colliding with nitrogen. A comparison of their results with the asymptotic cross sections of Ref. 14 was reported previously.[37] Those comparisons, together with the corrections to the asymptotes outlined here, and an analysis of the charge-state distributions obtained from Ref. 36, suggest that in this velocity regime the cross section for a change from charge q to charge $q+m$ (i.e., the loss of m electrons in a single collision) can be phenomenologically modeled by a relatively simple formula:

$$\sigma_{q,q+m}=\begin{cases}\dfrac{f}{2+f}(1-\delta_{\text{ex}})(\sigma_{\text{in, el}}+\sigma_{\text{in, in}}), & m=1\\[2ex] \dfrac{1}{2+f}\left(\tfrac{1}{2}\right)^{m-2}(1-\delta_{\text{ex}})(\sigma_{\text{in, el}}+\sigma_{\text{in, in}}), & m\geq 2\,.\end{cases} \tag{15}$$

For $f=5$, the m scaling given by Eq. (15) predicts relative multiple-electron-loss cross sections which agree to within about 10% of those in Ref. 36 at 13 MeV/amu for U^{10+} and U^{20+} ions. The agreement is generally about 20% over the 2–60-MeV/amu energy region for those ions. The recent experimental data of Horsdal-Pedersen and Larsen,[38] for simultaneous projectile-target ionization in

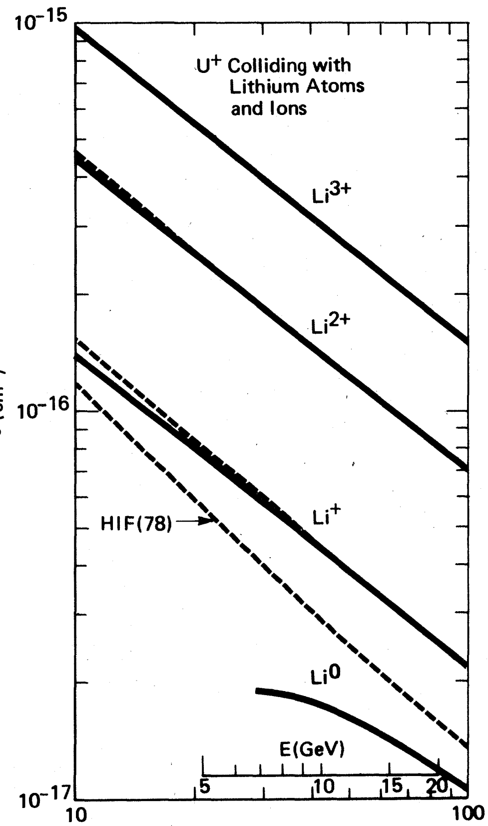

FIG. 1. Cross sections for the inelastic scattering of U^+ ions by lithium atoms and ions, which are upper bounds to the electron-stripping cross sections according to Eq. (4). Broken curves are cross sections given by retaining only the leading-order collision strength (in β^{-2} expansion) in Eqs. (5)–(7); solid curves include the second-order terms ($\gamma_{\mathrm{in,el}}$ and $\gamma_{\mathrm{in,in}}$). For neutral lithium targets these terms give rise to significant corrections in this velocity regime. That cross section is only shown for energies higher than that corresponding to the maximum; the expansion is apparently converging for $E/A \gtrsim 40$ MeV/amu. The leading-order term alone [labeled HIF(78), from Ref. 14] may give a sizable overestimate of the electron-stripping cross section at energies below that. For collisions with lithium ions, the second-order terms give only a small correction to the asymptote throughout this energy regime. However, the cross sections are significantly larger than for neutral lithium owing to the long-range contribution to the interaction from incomplete screening.

Xe-H collisions at ~0.5 MeV/amu, are also consistent with the m scaling given by Eq. (14) (for $m \leq 4$) if $f = 2$. The term δ_{ex} is a measure of the relative contribution of projectile excitation to the inelastic cross section. For the low-charge-state ions considered here ($q \leq Z/20$), δ_{ex} probably does not exceed 0.1–0.3, although

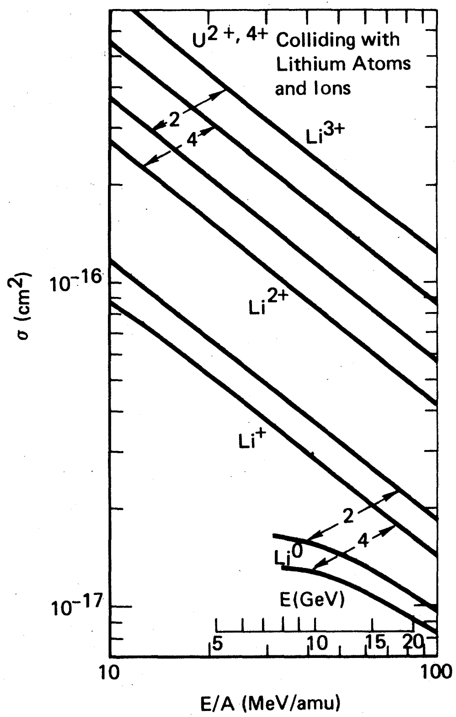

FIG. 2. Cross sections for the inelastic scattering of U^{2+} and U^{4+} ions by lithium atoms and ions, similar to those for U^+ shown in Fig. 1.

for higher initial charge states δ_{ex} may be larger.[19,37]

The simple model given by (15) is no more than that; it should not be taken as a claim to some fundamental scaling law. Nevertheless, it should be useful in assessing the importance of having detailed information on multiple electron-loss and excitation cross sections when estimating beam charge-state distributions in a heavy-ion ICF reactor concept.

B. Impact-ionization cross sections for lithium atoms and ions

As in the preceding section, the basic theory for the asymptotic Born approximation cross section has been described in previous work.[12] In this section we examine inelastic cross sections for the various charge states of lithium, which include target excitation as well as ionization, and for the cases of Li^0 and Li^{2+} we also compute the impact-ionization cross sections explicitly.[39] In the case of electron or proton impact on Li^0 in this velocity regime, the ionization cross section contributes a relatively small amount to the total inelastic cross section (~10%), owing primarily to the small ratio of $S(-1)_{\mathrm{ion}}/S(-1)$ for neutral lithium (see Table I). This suggested[14] that the cross sections for the inelastic scattering of Li^0 by fast complex ions may also be significantly overestimating the Born ionization cross sections.

The asymptotic form of the impact-ionization cross sections are similar to Eq. (7) since we are considering incident (U^{q+}) ions,[39] viz.,

$$\sigma(\mathrm{Li})_{\mathrm{ion}} = \sigma_{\mathrm{el,ion}} + \sigma_{\mathrm{in,ion}} = 4\pi a_0^2 \frac{\alpha^2}{\beta^2}\left(q^2 M_{\mathrm{ion}}^2 (\ln\beta^2\gamma^2 - \beta^2) + C_{\mathrm{el,ion}} + 2I_{\mathrm{in,ion}} + (\gamma_{\mathrm{el,ion}} + 2\gamma_{\mathrm{in,ion}})\frac{\alpha^2}{\beta^2}\right). \quad (16)$$

In Eq. (16), $q = F_0^{(1)}(0)$ is the net charge of the incident U^{q+} projectile, and $M_{\mathrm{ion}}^2 = S^{(2)}(-1)_{\mathrm{ion}}$ is the ionized final-state contribution to the -1 energy moment of the dipole oscillator strength distribution of the target lithium atom (or ion). The parameters $C_{\mathrm{el,ion}}$, $I_{\mathrm{in,ion}}$, $\gamma_{\mathrm{el,ion}}$, and $\gamma_{\mathrm{in,ion}}$ are analogous to those given in Table III and depend on atomic properties of both the incident projectile and target. In the case of Li^0 targets, we have calculated the corresponding collision strength parameters for excitation to discrete final states of the Li^0 and subtracted the sum of these from those values calculated via closure for all final states, i.e., the total inelastic collision strength parameters.[12] This is the same method as outlined in Ref. 39 for He targets. Results for U^+ and U^{4+} impact are summarized in Table IV, where we give explicitly the values of the momentum-transfer integrals $(\mathcal{G}_1 - \mathcal{G}_2)$ which dominate the collision strength parameters $C_{\mathrm{el,in}}$ and $C_{\mathrm{el,ion}}$. Table V gives abbreviated results for Li^{2+} ionization parameters, as well as the total inelastic parameters for several additional cases. For Li^{2+}, the ionization momentum-transfer integrals may be calculated directly, using previous results for the ionization contribution to the Li^{2+} incoherent scattering function.[19]

Table VI provides a summary of the collision strength parameters appearing in Eq. (16), which, together with the values of $S^{(2)}(-1)_{\mathrm{ion}}$ given in Table I, can be used to compute the asymptotic ionization cross section for U^+ and U^{4+} impact on Li^0 and Li^{2+}. For comparison we also give the corresponding total inelastic cross-section parameters $C_{\mathrm{el,in}}$ and $\gamma_{\mathrm{el,in}}$. These, together with the collision strengths $I_{\mathrm{in,in}}$ and $\gamma_{\mathrm{in,in}}$ given in Table III, and $S^{(2)}(-1)$ from Table I, can be used to compute the total cross section for impact excitation and ionization:

TABLE IV. Discrete final-state momentum-transfer integrals for the excitation of Li^0 by fast U^{q+} ions ($q = 1, 4$). Also given are total excitation collision strength parameters, total inelastic parameters, and, by taking the difference between these, the total ionization collision strength parameters.

Li final state (NL)	U^+ $I_{\mathrm{el},NL}$ or $(\mathcal{G}_1-\mathcal{G}_2)_{NL}$	U^+ $I_{\mathrm{in},NL}$	U^{4+} $I_{\mathrm{el},NL}$ or $(\mathcal{G}_1-\mathcal{G}_2)_{NL}$	U^{4+} $I_{\mathrm{in},NL}$
$2P$	(45.2)	8.25	(−106)	5.61
$3P$	(6.20)	0.478	(10.9)	0.340
$4P$	(2.01)	0.134	(2.78)	0.102
$5P$	(0.926)	0.0593	(1.16)	0.0452
$6P$	(0.507)	0.0318	(0.607)	0.0243
$7P$	(0.309)	0.0192	(0.360)	0.0147
NP ($N \geq 8$)	($100\ N^{-3}$)	$6.5\ N^{-3}$	($120\ N^{-3}$)	$5\ N^{-3}$
All NP	(56.1)	9.03	(−89.4)	6.18
$3S$	2.33	0.497	7.83	0.347
$4S$	0.649	0.127	1.80	0.0901
$5S$	0.279	0.0525	0.725	0.0376
NS ($N \geq 6$)	$30\ N^{-3}$	$6\ N^{-3}$	$80\ N^{-3}$	$4\ N^{-3}$
All NS	3.75	0.775	11.7	0.540
$3D$	3.89	0.803	12.7	0.563
$4D$	1.51	0.284	4.08	0.203
$5D$	0.739	0.133	1.86	0.0960
ND ($N \geq 6$)	$90\ N^{-3}$	$15\ N^{-3}$	$200\ N^{-3}$	$10\ N^{-3}$
All ND	7.61	1.47	21.9	1.03
Total excitation	(78.8)	11.3	(−22.2)	7.75
Total ionization	(1.32×10^3)	20.8	(1.39×10^3)	17.6
Total inelastic	(1.40×10^3)	32.1	(1.39×10^3)	25.4

$$\sigma(\mathrm{Li})_{\mathrm{ion}} \leq \sigma(\mathrm{Li})_{\mathrm{ex+ion}} = \sigma_{\mathrm{el,in}} + \sigma_{\mathrm{in,in}}$$

$$= 4\pi a_0^2 \frac{\alpha^2}{\beta^2}\left(q^2 S^{(2)}(-1)(\ln\beta^2\gamma^2 - \beta^2) + C_{\mathrm{el,in}} + 2I_{\mathrm{in,in}} + (\gamma_{\mathrm{el,in}} + 2\gamma_{\mathrm{in,in}})\frac{\alpha^2}{\beta^2}\right). \quad (17)$$

Figure 3 displays the cross sections given by Eq. (16) (solid curves) and Eq. (17) (broken curves) for U^{q+} impact on Li^0, Li^+, and Li^{2+}. Several observations on these cross sections should be mentioned. First, the ionization cross section for Li^0 is a substantial fraction of the total inelastic cross section, in contrast to the expectations mentioned in Ref. 14. For example, it contributes more than 88% in the case of U^+, and about 60% in the case of U^{4+}. The difference between this fraction for U^{q+} projectiles and that for protons or electrons, is due to the significantly different regions of momentum transfer typical for these different collisions. For projectiles which are pointlike on an atomic scale, these cross sections are dominated by low-momentum-transfer collisions. Hence, the ionization contribution to the inelastic cross section is roughly given by the ratio of the dipole limits of the transition strengths, $S(-1)_{\mathrm{ion}}/S(-1)$. For Li^0 this ratio is ~ 0.08. For collisions with heavy, low-charge-state ions, which are not pointlike on the atomic scale and have geometric cross sections comparable to (or larger than) the target particles, the typical momentum transfer is sizable. The collision cross section is dominated by interactions involving the atomic structure of the projectile, rather than the long-range Coulomb contribution to the interaction. As the charge state of the projectile is increased, the Born cross sections will eventually approach q^2 times the proton cross sections. This is not likely to occur until $q > 10$, however.[14]

TABLE V. Select momentum-transfer integrals $\mathcal{I}_1 - \mathcal{I}_2$ for U^{q+} ions ($q = 1, 2, 4$) on lithium atoms and ions; comparable results for U^+ and U^{4+} on Li^0 appear in Table IV. Also given for the case of Li^{2+} targets are the ionization contributions separately $(\mathcal{I}_1 - \mathcal{I}_2)_{\mathrm{ion}}$. These parameters, together with additional data from Table I, can be used to calculate the collision strength parameters $C_{\mathrm{el,in}}$ or $C_{\mathrm{el,ion}}$ as outlined in Refs. 12 or 39, respectively.

Projectile	Target	$\mathcal{I}_1 - \mathcal{I}_2$	$(\mathcal{I}_1 - \mathcal{I}_2)_{\mathrm{ion}}$
U^+	Li^+	7.00×10^2	
	Li^{2+}	$3.27 \pm 0.01 \times 10^2$	2.72×10^2
U^{2+}	Li^0	1.41×10^3	
	Li^+	7.02×10^2	
	Li^{2+}	3.28×10^2	2.72×10^2
U^{4+}	Li^+	7.13×10^2	
	Li^{2+}	3.32×10^2	2.74×10^2

Another result apparent from Fig. 3 is that the ionization cross sections are nearly independent of the uranium charge state (for $q \leq 4$), whereas the inelastic cross sections for U^+ and U^{4+} impact on Li^0 differ by a factor of 2. These results suggest that one can utilize the cross sections shown in Fig. 3 for U^{3+} impact and probably for any uranium ion of a low-charge state ($q \lesssim 6$).

C. Mean energy of collisionally produced electrons from Li^0

In addition to cross sections, the momentum-transfer formulation of the Born approximation is readily applicable to the computation of other properties of fast collisions. Recently, Kim and Cheng[40] have described calculations for the stopping power of partially stripped ions utilizing this approach. In this section we outline the calculation of a closely related quantity, the mean energy of electrons produced in the collisional ionization of Li^0 by fast U^+ and U^{4+} ions, and compare the results with those obtained for proton impact.

We start by considering two classes of stopping cross sections. Let $E_m^{(2)}$ denote the excitation energy of the mth state (discrete or in the continuum) of the Li^0 target atom, and define mean-excitation-energy cross sections according to

$$\langle \sigma_{\mathrm{el},m} E_m^{(2)} \rangle = \sum_m \sigma_{\mathrm{el},m} E_m^{(2)} , \quad (18)$$

$$\langle \sigma_{\mathrm{in},m} E_m^{(2)} \rangle = \sum_m \sigma_{\mathrm{in},m} E_m^{(2)} . \quad (19)$$

These are simply energy-weighted sums of the two types of target inelastic cross sections, corresponding to whether the incident projectile is scattered elastically (el) or inelastically (in). [These are two of the four possible contributions to the general stopping power formulas given by Kim and Cheng; see Eq. (4) of Ref. 40.]

With the aid of sum rules, Eqs. (18) and (19) may be evaluated for all inelastic collisions. Then by calculating the sum on the right-hand side for discrete states explicitly, and subtracting from the sum-rule results, one obtains the mean-ionization-energy cross sections. This is the same procedure utilized in the preceding section in order to obtain the ionization cross sections, only now each term is weighted by the corresponding excitation energy. Dividing this result by the ionization cross

TABLE VI. Collision strength parameters for the inelastic scattering of lithium atoms and ions by the impact of fast U^{q+} ions ($q=1,2,4$), denoted by $C_{el,in}$ and $\gamma_{el,in}$. Together with the parameters $I_{in,in}$ and $\gamma_{in,in}$ given in Table III and the values of $S^{(2)}(-1)$ for the different charge states of lithium from Table I, the total cross section for collisional excitation and ionization of the lithium can be obtained via Eq. (17). Also given are the corresponding parameters for the ionization alone of the Li^0 and Li^{2+}, denoted by $C_{el,ion}$, $I_{in,ion}$, $\gamma_{el,ion}$, and $\gamma_{in,ion}$. The impact-ionization cross sections are given similiarly by Eq. (16).

Projectile	Target	$C_{el,in}$	$C_{el,ion}$	$I_{in,ion}$	$\gamma_{el,in}$	$\gamma_{el,ion}$	$\gamma_{in,ion}$
U^+	Li^0	1.49×10^3	1.32×10^3	20.8	-6.50×10^3	-6.49×10^3	-2.95×10^3
	Li^+	7.02×10^2			-4.38×10^3	-4.35×10^3	-9.26×10^2
	Li^{2+}	3.28×10^2	2.72×10^2	2.54	-2.20×10^3	-2.17×10^3	-2.22×10^2
U^{2+}	Li^0	1.76×10^3			-6.61×10^3	-6.60×10^3	-2.93×10^3
	Li^+	7.11×10^2			-4.49×10^3	-4.45×10^3	-9.18×10^2
	Li^{2+}	3.31×10^2	2.73×10^2	2.45	-2.27×10^3	-2.22×10^3	-2.18×10^2
U^{4+}	Li^0	2.79×10^3	1.46×10^3	17.6	-6.78×10^3	-6.76×10^3	-2.92×10^3
	Li^+	7.47×10^2			-4.65×10^3	-4.59×10^3	-9.08×10^2
	Li^{2+}	3.44×10^2	2.77×10^2	2.29	-2.36×10^3	-2.28×10^3	-2.14×10^2

sections of the previous section then yields the mean energy of the electrons produced by the collisional ionization of the Li^0.

Since the more general energy-loss problem is treated in detail by Kim and Cheng,[40] we give here selected results in order to relate our notation[41] to that work. Specifically, the sum over all final states (m) of Eqs. (18) and (19) may be written as

$$\langle \sigma_{el,m} E_m^{(2)}\rangle = 4\pi a_0^2 \frac{\alpha^2}{\beta^2}\left[(Z_N^{(1)2}+q^{(1)2})Z_e^{(2)}\left(\ln\frac{4\beta^2\gamma^2}{\alpha^2}-\beta^2-\ln G_f^{(1)}\right)-2q^{(1)2}L^{(2)}(0)\right], \quad (20)$$

$$\langle \sigma_{in,m} E_m^{(2)}\rangle = 4\pi a_0^2 \frac{\alpha^2}{\beta^2}\left[Z_e^{(1)}Z_e^{(2)}\left(\ln\frac{4\beta^2\gamma^2}{\alpha^2}-\beta^2-\ln G_s^{(1)}\right)\right], \quad (21)$$

to leading order in an expansion in β^{-2}; $Z_N^{(1)}$, $Z_e^{(1)}$, and $q^{(1)}$ denote the nuclear charge, electron charge, and net charge of the incident projectile, respectively. Similarly, $Z_e^{(2)}$ is the number of electrons on the target atom. (These follow the notation of Ref. 12.) The parameters $\ln G_f^{(1)}$ and $\ln G_s^{(1)}$ are properties of the projectile and may be calculated from the elastic form factors and incoherent scattering functions[40] of U^{q+} ions. The parameter $L^{(2)}(0)$ is the logarithmic energy moment of the dipole-oscillator-strength distribution for the target particle. For Li^0, Dehmer *et al.*[21] report a value of 2.749 calculated within the context of the Herman-Skillman model, which is the value we adopt here.[42]

Table VII summarizes results for $\ln G_f$ and $\ln G_s$ and the mean-ionization energies for U^+ and U^{4+}, and H^+ impact on Li^0. The typical mean-ionization energy for these low-charge-state uranium ions is in the keV range, whereas for proton impact it is several tens of eV. The difference is again due to the fact that ionizing collisions with these heavy, structured ions involve momentum transfers significantly larger than for structureless particles. As the charge state of the U^{q+} ion is increased these mean energies will approach those for H^+ impact. There are significant differences as well in the kinematics of U^{q+} and H^+ impact which must be considered in assessing the implications of these results. Note also that these mean energies are not related in any simple way to the effective excitation energy as defined by Kim and Cheng,[40] but are related to the mean kinetic energies of collisionally produced electrons.

The temperature of electrons utilized to neutralize the space-charge force of an ion beam plays an important role in the effectiveness of the neutralization during propagation in an ICF reactor.[44] If these neutralizing electrons are collisionally produced from a background gas by the impact of the ions in the beam, the results summarized in Table VII suggest that their initial kinetic energies (i.e., prior to degradation) will be substantially higher than in the more familiar case of proton (or electron) impact.

III. SUMMARY

We have presented Born calculations for the cross sections of fast U^{q+} ions colliding with lith-

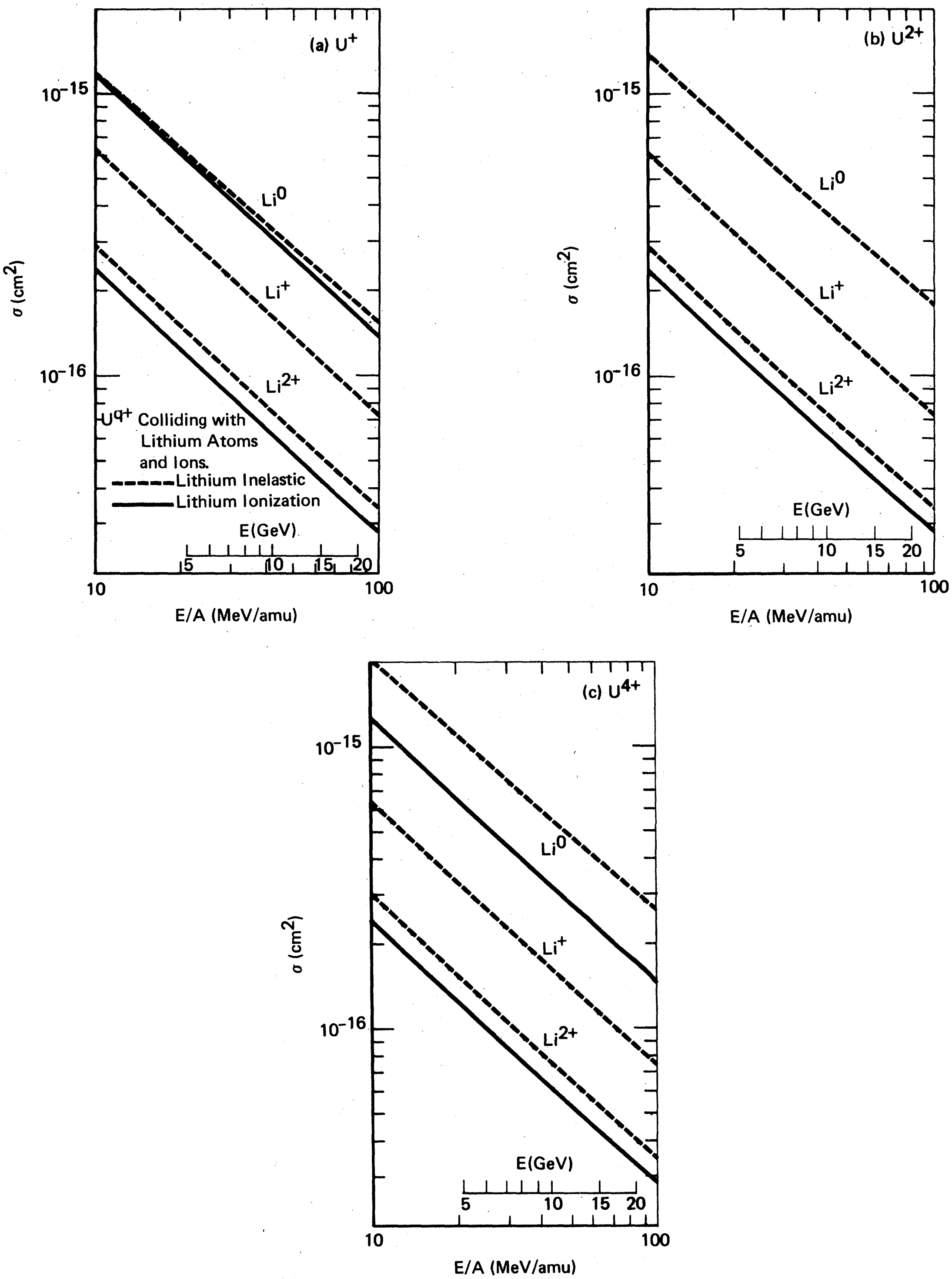

FIG. 3. (a) Impact-ionization cross sections for Li^0 and Li^{2+} due to fast U^+ ions (solid curves), and cross sections for the total inelastic scattering (excitation and ionization) of lithium atoms and ions in fast collisions with U^+ (broken curves). These results show that ionization accounts for 75% or more of the total inelastic cross sections for singly charged uranium colliding with Li^{2+}, and for over 88% in collisions with Li^0. (b) Similar results for U^{2+} impact and (c) U^{4+} impact. As the charge state of the uranium ion increases, excitation of the Li^0 and Li^{2+} becomes increasingly important as a contributor to the total inelastic-scattering cross section. In the case of U^{4+} impact, ionization still accounts for over 75% of that cross section for Li^{2+} targets, but has dropped to 55–62% for Li^0 targets.

TABLE VII. Numerical values for the integrals $\ln G_F$ and $\ln G_S$ for U^{q+} ions ($q=1,2,4$) as defined in Ref. 40 and mean energies of ionization $\overline{E_{\text{ion}}^{(2)}}$, for Li^0 due to the impact of fast U^+, U^{4+}, and H^+ ions at 10 and 100 MeV/amu. The mean kinetic energy of the ionized electrons (with respect to the final-state center of mass of the Li^+-e^- system) is given by $\overline{E_{\text{ion}}^{(2)}} - E_B^{(2)}$, where $E_B^{(2)}$ is the ionization potential of lithium (0.4 Ry).

Ion	$\ln G_F$	$\ln G_S$	$\overline{E_{\text{ion}}^{(2)}}$ (Ry) 10 MeV/amu	100 MeV/amu
U^+	4.52	3.83	59	100
U^{2+}	4.51	3.87		
U^{4+}	4.50	3.96	50	88
H^+	0	0	5.3	6.2

ium atoms and ions. The emphasis has been on obtaining reasonable approximations to the electron-stripping cross sections in the 10–20 GeV energy regime (40–80 MeV/amu). Since these are predominantly outer-shell collision processes of the uranium, and the target particles are low Z, the Born approximation should provide a reliable basis for calculating these cross sections at these energies. Corrections to the asymptotic cross sections examined here are significant for collisions with neutral Li^0, but for $E \geq 8$ GeV the two-term expansion in β^{-2} should give a good approximation to Born cross sections. We anticipate that the cross sections in Figs. 1 and 2 (solid curves) should provide reliable (factor of 2) estimates of the U^{q+} ($q=1,2,4$) electron-stripping cross sections.

Cross sections for the impact ionization of lithium due to fast U^{q+} ions have also been reported. We have explicitly examined the excitation contribution to the total inelastic cross sections and found it less significant (< 50%) than in the case of electron or proton impact (~90%). While our basic approach for handling the electronic structure is consistent with experiments for light ions,[39,43] these cross sections for low-charge-state heavy ions are likely to be larger than actual impact-ionization cross sections. Non-Born corrections can be significant in this type of collision, which is dominated by the elastic scattering of a heavy particle carrying a large number of electrons.[45]

Our results for the mean energy of electrons produced in the impact ionization of Li^0 by U^+ and U^{4+} show substantial differences from the case of proton impact. We can anticipate corrections to this from non-Born affects, similar in origin to those mentioned above, but it seems apparent that order-of-magnitude differences between the cases of electron or proton impact and low-q, heavy ions will remain.

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