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The role of charge-exchange processes in probing hydrogen plasma with a heavy ion beam

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ABSTRACT

Charge-changing processes of low-charged ions, used in hydrogen plasma probing by the heavy ion beam probe method, are considered. Along with the ionization of beam ions by plasma electrons and protons, the charge-exchange processes of ions on H atoms and protons are also studied. It is shown that charge exchange of beam ions on plasma protons and H atoms, which is rarely taken into account, plays an important role in beam–plasma interaction. New data on the cross sections and rates of ionization and charge-exchange processes are presented for Tl^+ and Tl^{2+} ions, which are frequently used for plasma diagnostics. Calculations are performed for hydrogen plasma temperatures T_e = 1 eV–10 keV and densities $N_e = 10^{12}$–10^{14} cm^{-3} at relatively low and high ion-beam velocities v_b = 0.2 and 1.0 a.u., respectively. Special attention is paid to the determination of the electron temperatures at which the charge-exchange processes on H atoms and protons are important. Multiple ionization of beam ions by plasma electrons and protons is briefly discussed.

I. INTRODUCTION

The interaction of ion beams with plasma particles is of practical significance in a number of areas, such as production of radioactive ions, determination of ion stopping power, and plasma diagnostics, as well as playing an important role in a variety of astrophysical phenomena. The heavy ion beam probe (HIBP) method is one of the main techniques for plasma particle diagnostics, enabling measurements of important plasma parameters such as electron density and temperature and electric and magnetic plasma potentials (see, e.g., Refs. 1 and 2). Plasma probing is carried out using beams of low-charged heavy ions such as Cs^+, Tl^+, and Au^+ with a beam energy ranging from several hundred keV to tens of MeV for plasma diagnostics in the temperature range T = 1 eV–5 keV (see, e.g., Ref. 1). When an ion beam collides with a hydrogen plasma, the intensity and energy of secondary doubly charged ions are usually determined by the rates of one- and two-electron ionization by plasma electrons and protons.[3–5] Charge exchange of incident ions on H atoms and protons are rarely taken into account, owing to the lack of information on charge-exchange cross sections in a wide energy range required to determine the rates of these processes.[3,5,6]

The aim of the present work is to investigate the role of charge exchange in hydrogen-plasma HIBP diagnostics. Charge-exchange processes of Tl^+ and Tl^{2+} ions on H atoms and protons are studied for plasma temperatures T_e = 1 eV–10 keV and densities $N_e = 10^{12}$–10^{14} cm^{-3}. Two cases of relatively low and high ion-beam velocities v_b = 0.2 and 1.0 a.u., respectively, are considered, where the atomic unit of velocity is 1 a.u. $\simeq 2.2 \times 10^8$ cm/s. It is shown that charge exchange plays a substantial role in plasma diagnostics, depending on the electron temperature and ion-beam velocity.

II. IONIZATION AND CHARGE-EXCHANGE PROCESSES

In the HIBP method, the attenuation of the primary and secondary ion beams depends mainly on the rates (in units of s^{-1}) of the charge-changing processes with plasma particles:

$$N\langle v\sigma\rangle = N\int_0^\infty v\sigma(v)F(v, v_b, T)\,dv, \tag{1}$$

where N and T are the density and temperature of plasma particles, respectively, $\sigma(v)$ is the effective cross section, $\langle v\sigma\rangle$ is the rate coefficient in units of cm^3/s, v_b is the ion-beam velocity, and $F(v, v_b, T)$ is the velocity distribution function of plasma particles (electrons, protons, and H atoms). In a equilibrium hydrogen plasma, the temperatures of electrons, protons, and H atoms are equal, $T_e = T_p = T_H$, as are the densities of electrons and protons, $N_e = N_p$. The hydrogen density N_H depends strongly on the parameters T_e and N_e and is usually found by solving the kinetic equations in a certain radiative-collisional plasma model (see, e.g., Refs. 7 and 8).

The velocity distribution of plasma particles in the ion center-of-mass system is described by the "shifted" Maxwellian function[9]

$$F(v, v_b, T) = \left(\frac{\mu}{2\pi kT}\right)^{1/2} \frac{v}{v_b} \left\{ \exp\left[-\frac{\mu}{2kT}(v - v_b)^2\right] - \exp\left[-\frac{\mu}{2kT}(v + v_b)^2\right]\right\}, \quad (2)$$

where $v = |\mathbf{v}_b - \mathbf{V}|$ is the velocity of ions in the beam relative to the velocity V of plasma particles, μ is the reduced mass of the colliding particles, and k is Boltzmann's constant. At zero ion velocity, $v_b = 0$, the function (2) turns into the "usual" Maxwellian function

$$F(v, v_b \to 0, T) = 4\pi v^2 \left(\frac{\mu}{2\pi kT}\right)^{3/2} \exp\left(-\frac{\mu v^2}{2kT}\right). \quad (3)$$

The function (2) is normalized to unity for all values of v_b and T:

$$\int_0^\infty F(v, v_b, T)\, dv = 1. \quad (4)$$

In the interaction of a beam of low-charged positive ions X^{q+} with a hydrogen plasma, the following charge-changing processes play the main role:

(i) multielectron (ME) ionization by electrons:

$$X^{q+} + e^- \to X^{(q+n)+} + (n+1)e^-, \quad n \ge 1, \quad (5)$$

(ii) ME ionization by protons:

$$X^{q+} + p \to X^{(q+n)+} + p + ne^-, \quad n \ge 1, \quad (6)$$

(iii) charge exchange on H atoms:

$$X^{q+} + \mathrm{H} \to X^{(q-1)+} + p, \quad (7)$$

(iv) charge exchange on protons:

$$X^{q+} + p \to X^{(q+1)+} + \mathrm{H}, \quad (8)$$

where q is the ion charge and n is the number of ejected electrons.

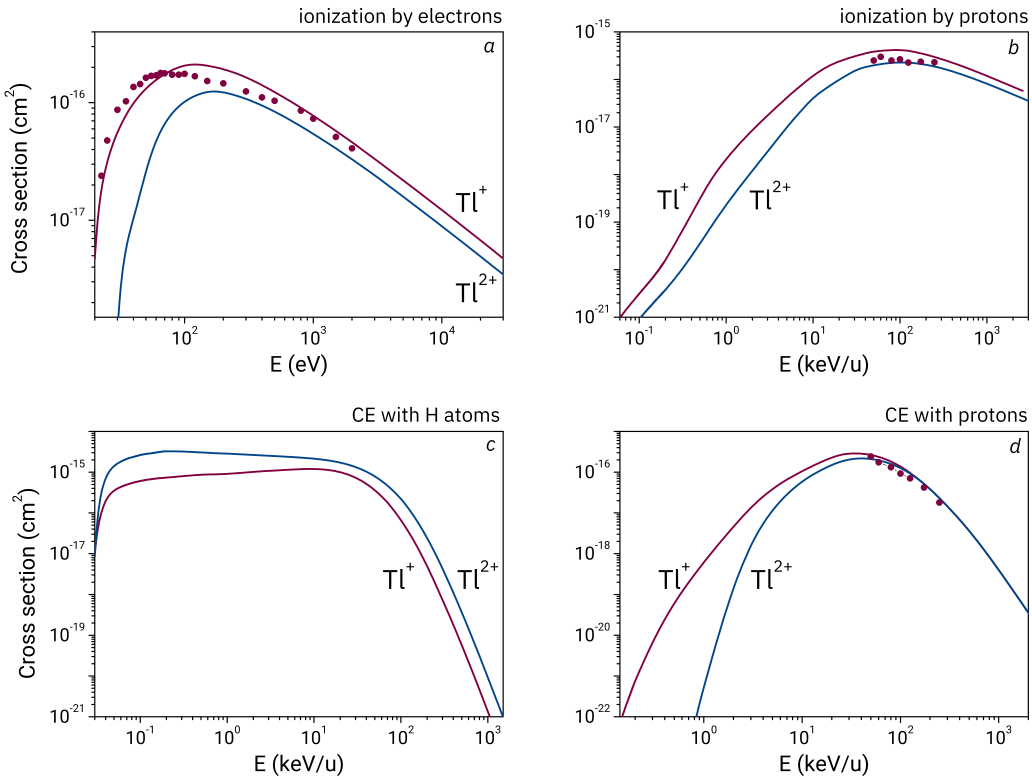

FIG. 1. One-electron cross sections for ionization and charge exchange of Tl^+ and Tl^{2+} ions in collision with plasma particles. (a) Electron-impact ionization: circles, experiment[11] for Tl^+; solid curves, calculations using the ATOM code.[10] (b) Ionization by protons: circles, experiment[12] for Tl^+; solid curves, calculations using the ARSENY[13] and RICODE-M[14] codes. (c) Cross sections for charge-exchange on H atoms calculated using the ARSENY and CAPTURE codes.[15] (d) Cross sections for charge exchange on protons: circles, experiment[12] for Tl^+; solid curves, calculations using the ARSENY and CAPTURE codes.

III. CALCULATIONS OF IONIZATION AND CHARGE-EXCHANGE CROSS SECTIONS

The results of numerical calculations of one-electron ionization and charge-exchange cross sections of the processes (5)–(8) for Tl^+ $(5p^6 5d^{10} 6s^2)$ and $Tl^{2+}(5p^6 5d^{10} 6s^1)$ ions are presented in Fig. 1 in comparison with available experimental data. The contribution of ME ionization processes of ions by electrons and protons is discussed in Sec. V.

Calculations of ionization cross sections were carried out using the ATOM code[10] in the Coulomb–Born approximation with account taken of electron exchange. The corresponding cross sections are shown in Fig. 1(a) in comparison with experimental data[11] for Tl^+ ions. Figure 1(b) shows the cross sections for one-electron ionization by protons in comparison with experimental data for Tl^+ ions.[12] Two different codes were adopted to calculate proton-impact ionization cross sections: at low energies, the ARSENY code[13] based on the hidden crossings method in the adiabatic approximation was applied, while at high energies, the RICODE-M code[14] using the relativistic Born approximation with relativistic (magnetic) interaction between colliding particles was applied. The two cross sections connect smoothly at around 70–80 keV/u, where the adiabatic approximation becomes inapplicable and the relativistic Born approximation comes into play. These energies correspond approximately to the position of the cross section maximum. Calculated cross sections are shown in Fig. 1(b). The charge-exchange cross sections of Tl^+ and Tl^{2+} ions in collisions with H atoms (7) and protons (8) were obtained using the ARSENY and CAPTURE[15] codes and are presented in Figs. 1(c) and 1(d), respectively, in comparison with experimental data for the charge exchange of Tl^+ ions on protons[12] [Fig. 1(d)]. The CAPTURE code is based on the Brinkman–Kramers approximation using the normalized single-electron capture probabilities. Detailed descriptions of the codes mentioned here and their applications are presented in Ref. 16.

All calculated cross sections of thallium ions, presented in Fig. 1, are in good agreement with available experimental data for Tl^+ ions. At high energies, the cross sections for both ions are similar owing to the small contribution of the outer 6*s* electron of thallium ions, since the more inner-shell electrons start to play a role with increasing energy. Charge-exchange cross sections in collisions with H atoms [Fig. 1(c)] are quite large, especially for Tl^{2+} ions, owing to the small resonance defect $\Delta E_{\rm res}$ = 4.17 eV of the reaction. The cross sections for charge-exchange on protons [Fig. 1(d)] are very close to each other at high energies, where the main contribution comes from the capture of inner-shell target electrons,[17] whose binding energies for Tl^+ and Tl^{2+} ions have very close values. All these features of the ionization and charge-exchange cross sections manifest themselves in the rates of the processes as functions of plasma electron temperature T_e.

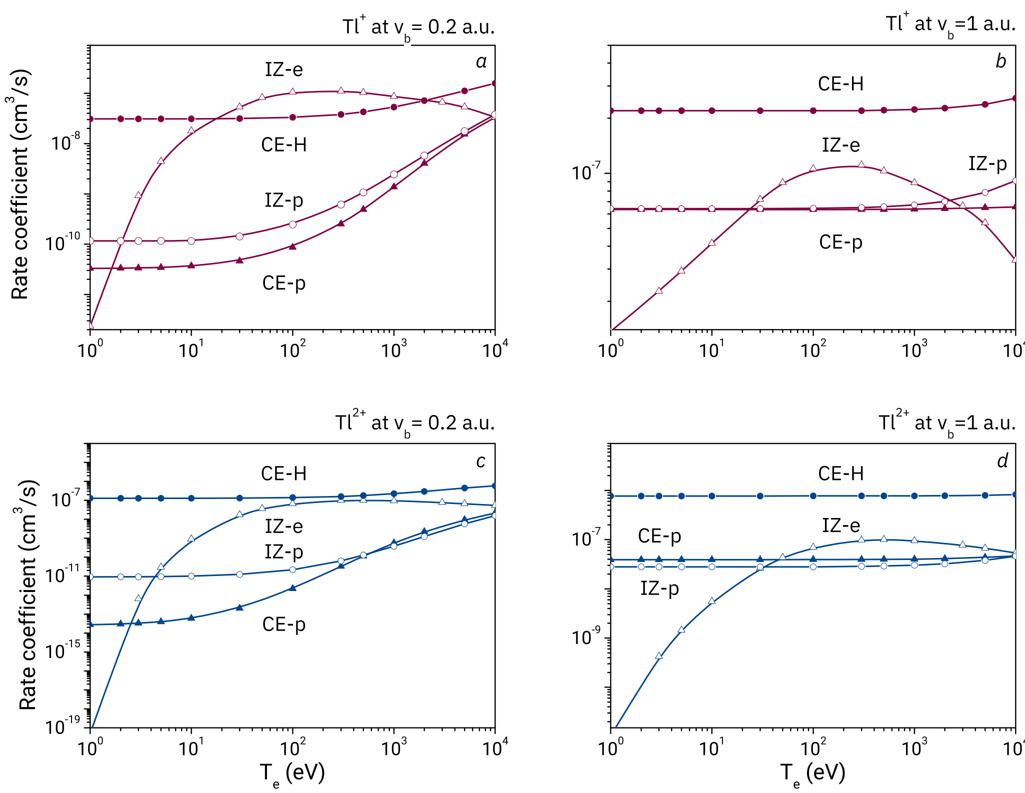

FIG. 2. Rate coefficients $\langle v\sigma \rangle$ of one-electron ionization and charge exchange for thallium ions as functions of plasma electron temperature T_e. (a) and (b) $\langle v\sigma \rangle$ values of Tl^+ ions at ion-beam velocity v_b = 0.2 a.u. and v_b = 1.0 a.u.; (c) and (d) $\langle v\sigma \rangle$ values of Tl^{2+} ions at v_b = 0.2 a.u. and 1.0 a.u. The results labeled IZ-e and IZ-p are for ionization by electrons and protons, respectively, and those labeled CE-H and CE-p are for charge-exchange on H atoms and protons, respectively.

IV. RATE COEFFICIENTS OF CHARGE-CHANGING PROCESSES FOR THALLIUM IONS IN HYDROGEN PLASMA

The rate coefficients $\langle v\sigma\rangle$ for ionization and charge-exchange processes for Tl^{+} and Tl^{2+} ions in a hydrogen plasma are presented in Fig. 2 as functions of electron temperature in the range T_e = 1 eV–10 keV. The data were obtained using the calculated cross sections shown in Fig. 1 and a shifted Maxwellian function (2) at two beam velocities v_b = 0.2 and 1.0 a.u., corresponding to relatively low and high energies of the thallium ion beam: $E_b \approx 204$ and 5100 keV, respectively. The figure shows the leading role of charge exchange on H atoms for both Tl^{+} and Tl^{2+} ions over the entire temperature range, especially at high ion-beam energies.

The coefficients $\langle v\sigma\rangle$ for Tl^{+} ions are shown in Fig. 2. At a beam velocity v_b = 0.2 a.u. [Fig. 2(a)], the rate coefficient for charge exchange on H atoms (CE-H) is comparable to that for ionization by electrons (IZ-e) at all temperatures except for the range T_e = 1–10 eV, where the CE-H coefficient significantly exceeds the IZ-e coefficient. At a large velocity v_b = 1.0 a.u. [Fig. 2(b)], the CE-H coefficient is the largest, the IZ-e coefficient changes slightly, and the IZ-p and CE-p coefficients become of the same order and comparable to the IZ-e coefficient. A similar situation with regard to the charge-changing rate coefficients occurs for Tl^{2+} ions [Figs. 2(c) and 2(d)].

V. ROLE OF CHARGE-EXCHANGE PROCESSES

The influence of each atomic process in a plasma is determined by the *rates* of the processes, $N\langle v\sigma\rangle$, rather than by the rate coefficients, where N is the density of plasma particles. For ionization by electrons and protons, and charge exchange on protons, the densities N are the same, $N_e = N_p$, but the density of H atoms $N_{\rm H}$ (and therefore, the CE-H rates) depends strongly on the electron temperature T_e and electron density N_e.

The H-atom density $N_{\rm H}$ in a hydrogen plasma with electron temperature T_e in the range 0.5–50 eV and electron density N_e in the range 10^{12}–10^{22} cm^{-3}, calculated in the radiative-collisional model using the FLYCHK code,[8] is given in Ref. 18. For the values of the electron density $N_e = 10^{12}$–10^{14} cm^{-3} considered in the present paper, the density $N_{\rm H}$ from Ref. 18 is shown in Fig. 3. As can be seen, $N_{\rm H}$ increases with increasing electron density N_e, but decreases rapidly with increasing electron temperature T_e in the range T_e = 1–10 eV. The sharp decrease in $N_{\rm H}$ with increasing electron temperature greatly reduces the temperature range in which the charge-exchange rates $N\langle v\sigma\rangle$ are important, although the corresponding rate coefficients $\langle v\sigma\rangle$ are very large.

To estimate the plasma temperature range in which charge exchange on H atoms makes a significant contribution to the total rate of beam attenuation, we assume that the ratio of the charge-exchange (CE-H) rate to the ionization (IZ-e) rate is more than 0.5, i.e.,

$$\frac{N_{\rm H}\langle v\sigma\rangle_{\rm CE-H}}{N_e\langle v\sigma\rangle_{\rm IZ-e}} \geq 0.5, \quad (9)$$

which imposes the following condition on the H-atom density $N_{\rm H}$:

$$N_{\rm H} \geq 0.5\frac{N_e\langle v\sigma\rangle_{\rm IZ-e}}{\langle v\sigma\rangle_{\rm CE-H}}. \quad (10)$$

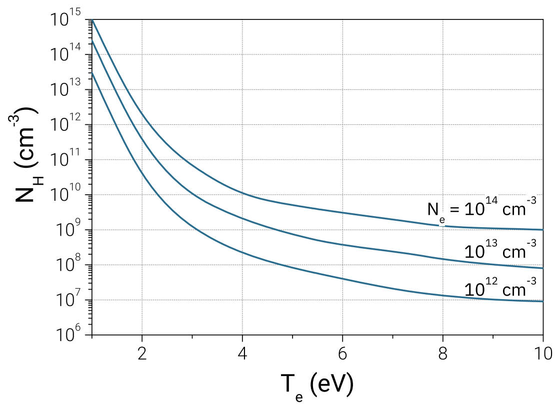

FIG. 3. Hydrogen-atom density $N_{\rm H}$ as a function of electron temperature T_e at electron densities $N_e = 10^{12}$, 10^{13}, and 10^{14} cm^{-3}.

Figure 4 shows the dependence of $N_{\rm H}$ on electron temperature T_e for thallium ions at ion-beam velocities v_b = 0.2 a.u. and v_b = 1.0 a.u., where the ascending curves correspond to the lower limits of the hydrogen density $N_{\rm H}$ in (10) and the descending ones to the densities $N_{\rm H}$ from Fig. 3. All the curves are plotted for electron densities $N_e = 10^{12}$–10^{14} cm^{-3}. The intersection points of the curves, marked by arrows, show the maximum electron temperatures at which the ratios of the charge-exchange (CE-H) rates to the ionization (IZ-e) rates are greater than 0.5. According to Fig. 4, the CE-H processes play an important role at low plasma temperatures $T_e \approx$ 1–3.5 eV. The contribution of the CE-p rate depends strongly on the ion-beam velocity: at v_b = 0.2 a.u., the contribution is large if the plasma temperature T_e > 2 keV, whereas at high velocity v_b = 1.0 a.u., the contribution of the CE-p rate is significant at almost all temperatures and is comparable to the contribution of the IZ-p rate.

VI. INFLUENCE OF MULTIELECTRON IONIZATION BY ELECTRONS AND PROTONS

In the preceding sections, the processes of one-electron ionization in the interaction of an ion beam with plasma electrons and protons have been considered. Now we estimate the possible contribution of multielectron (ME) ionization of Tl^{+} and Tl^{2+} ions by electron and proton impact. In recent work,[19] the contribution of ME ionization by electrons to the total ionization rates of beam ions in a plasma was studied as a function of the plasma electron temperature T_e and ion-beam velocity v_b. It was shown that the contribution of ME processes to the total ionization rate increases with increasing velocity v_b and that the maximum contribution $R_{\rm max}$ of ME ionization by plasma electrons is reached at high temperatures T_e and high velocities v_b. The value of $R_{\rm max}$ is given by the ratio

$$R_{\rm max} = \left[\frac{\sum_{n\geq 2}\langle v\sigma_n(v)\rangle}{\sum_n\langle v\sigma_n(v)\rangle}\right]_{\rm max} = \frac{\sum_{n\geq 2}\sigma_n(v\to\infty)}{\sigma_{\rm tot}(v\to\infty)}, \quad (11)$$

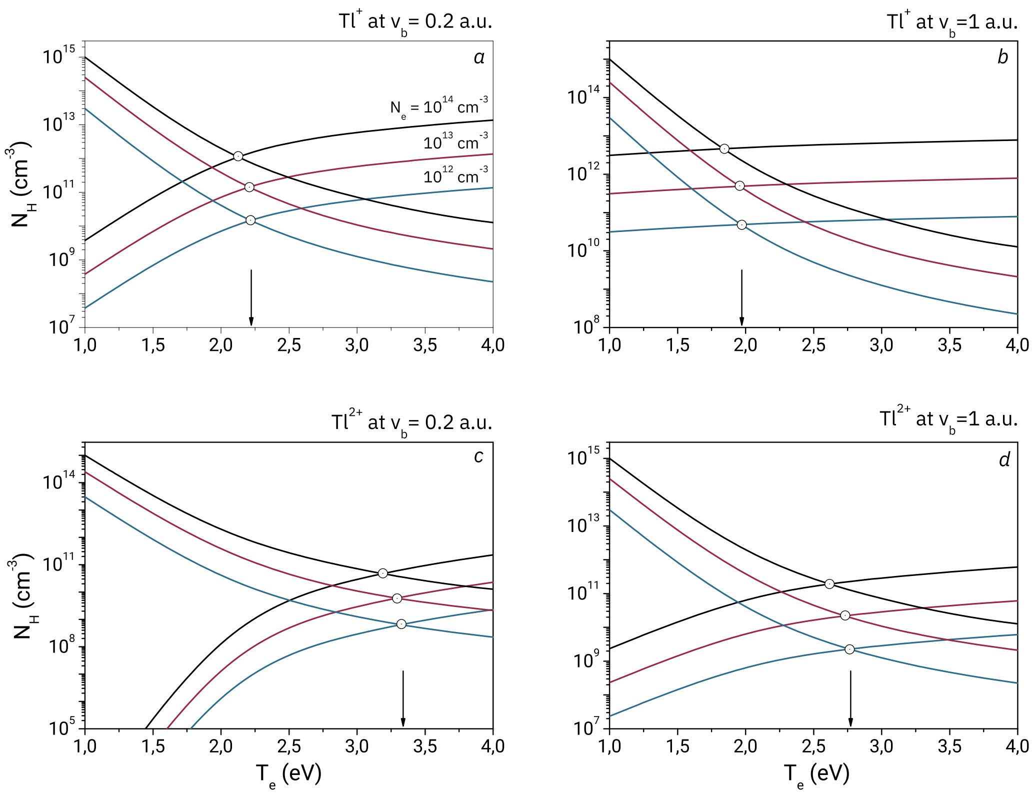

FIG. 4. Dependence of the H-atom density N_H on electron temperature T_e at electron densities $N_e = 10^{12}$, 10^{13}, and 10^{14} cm^{-3} and ion-beam velocities $v_b = 0.2$ and 1.0 a.u. The decreasing curves are from the calculation in Ref. 18, while the increasing curves are the lower limits of the density N_H from Eq. (10). The arrows indicate the maximum electron temperatures at which the CE-H rates should be accounted for as well as the IZ-e rates.

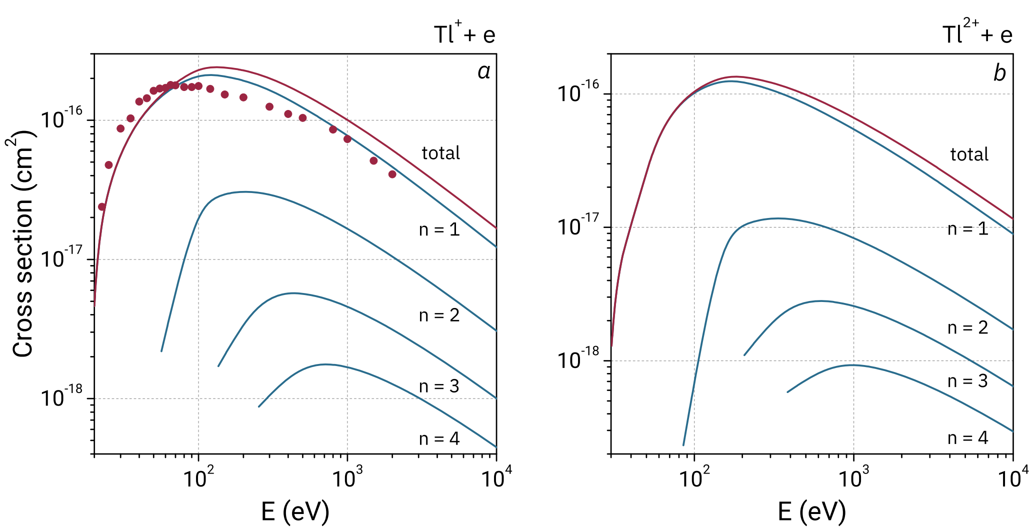

FIG. 5. ME ionization cross sections (for $n = 1$–4 electrons) by electron impact of (a) Tl^{+} and (b) Tl^{2+} ions as functions of electron energy: symbols, experiment;[11] solid curves, calculations for $n = 1$ using the ATOM code and for $n \geq 2$ using analytical formulas from Ref. 20, the curves marked "total" are the total cross sections.

where $\sigma_n(v \to \infty)$ is the cross section for n-electron ionization by electrons and $\sigma_{\rm tot}(v \to \infty)$ is the total (summed over all n) cross section. It follows from (11) that

$$\sigma_{\rm tot}(v) = \frac{\sigma_1(v)}{1 - R_{\max}}, \quad v \to \infty, \tag{12}$$

where $\sigma_1(v)$ is the one-electron ionization cross section. If the contribution of ME ionization is small ($R_{\max} \to 0$), then $\sigma_{\rm tot} \approx \sigma_1$, but with increasing $R_{\max}$, the total cross section $\sigma_{\rm tot}$ becomes much larger than σ_1 ($\sigma_{\rm tot} \gg \sigma_1$), and the use of just the one-electron cross section σ_1 can lead to a significant error.

Figure 5 shows the results of the present calculations of the cross sections for one-electron ($n = 1$) and ME ($n = 2, 3, 4$) ionization of Tl^+ and Tl^{2+} ions by electron impact as functions of electron energy. For $n = 1$, the cross sections were calculated using the ATOM code and for $n \geq 2$ using analytical approximations from Ref. 20. Based on the results obtained in Ref. 20, the maximum contributions $R_{\max}$ in (11) are estimated as $R_{\max} \sim 40\%$ for Tl^+ and $R_{\max} \sim 25\%$ for Tl^{2+}, i.e., according to (12), the maximum increases in the total ionization rate (IZ-e) coefficients for Tl^+ and Tl^{2+} ions due to ME ionization are about 1.7 and 1.3 times, respectively. There are no experimental data on cross sections for ME ionization of low-charged ions by protons, but data are available for *neutral* atoms (see, e.g., Refs. 20 and 21). It has been shown[21] that at asymptotic energies, experimental cross sections for ME ionization of Ne, Ar, Kr, and Xe atoms by protons and electrons are close to each other and make approximately equal maximum contributions to the total ionization cross sections. If we assume that low-charged ions have the same property as neutrals, i.e., that $R_{\max}$ values for ionization by protons and electrons are approximately equal, then the maximum contribution to ionization of low-charged thallium ions by proton impact can be estimated as $R_{\max} \approx 30\%$ according to the results for ME ionization by electrons shown in Fig. 5.

VII. CONCLUSIONS

The processes of ionization and charge exchange of low-charged ions in hydrogen plasma have been considered. Numerical calculations of cross sections $\sigma(v)$ and rates $N\langle v\sigma(v)\rangle$ of these processes have been performed for Tl^+ and Tl^{2+} ions with a shifted Maxwellian function at plasma temperatures $T_e = 1$ eV–10 keV, densities $N_e = 10^{12}$–10^{14} cm^{-3}, and ion-beam velocities $v_b = 0.2$ and 1.0 a.u.

It has been shown that charge exchange on H atoms plays an important role at low plasma temperatures $T_e \approx 1$–3.5 eV, regardless of the ion beam velocity. The charge exchange of beam ions on protons depends significantly on the ion-beam velocity v_b: at a low velocity $v_b = 0.2$ a.u., it plays a role only at high plasma temperatures $T_e > 2$ keV, but at a high velocity $v_b = 1.0$ a.u., it is important at all temperatures and makes a contribution to the total attenuation rate comparable to those of proton-ionization processes. Multielectron ionization of beam ions by electrons and protons can increase the corresponding rates by up to about 30% depending on the behavior of multielectron cross sections at high collision energies. Finally, we note that all the methods adopted here for thallium ions, and the conclusions obtained, are also applicable to other probe ions (Rb^+, Cs^+, W^+, etc.) used in beam diagnostics of plasma devices.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Inga Yu. Tolstikhina: Conceptualization (equal); Data curation (equal); Investigation (equal); Software (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **V. P. Shevelko**: Conceptualization (equal); Data curation (equal); Investigation (equal); Software (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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