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Charge-exchange-produced K -shell x-ray emission from Ar^{16+} in a tokamak plasma with neutral-beam injection

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High-resolution spectroscopy of a hot tokamak plasma seeded with argon ions and interacting with an energetic, short-pulse neutral hydrogen beam was used to obtain a high-resolution K -shell x-ray spectrum formed solely by charge exchange. The observed K -shell emission of Ar^{16+} is dominated by the intercombination and forbidden lines, providing clear signatures of charge exchange. Results from an *ab initio* atomic cascade model provide excellent agreement, validating a semiclassical approach for calculating charge-exchange cross sections.

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X-ray emission produced by charge exchange between highly charged ions and neutral atoms has generated strong interest since the unexpected discovery of x-ray emission from comets [1,2]. Charge exchange has now been recognized as the possible x-ray production mechanism in many other emitters such as Jupiter's aurora, the atmosphere of Mars, the extended galactic ridge emission, and hot gas from supernova remnants contacting neutral clouds [3–7]. It is a diagnostic for mass loss of stars [8] and may contribute to the soft-x-ray background in the heliosphere [9].

Fundamental principles involved in charge exchange have been studied by sophisticated experimental methods that provide full accounting of the collision products, such as the cold-target recoil-ion momentum spectroscopy method [10–12]. However, only a few studies have focused on x-ray emission [13]. As a result, x-ray spectral modeling predictions are still in flux and more laboratory data are direly needed. Predictions for the K -shell emission of heliumlike ions, for example, differ in which of the four possible emission lines is the strongest. Early predictions favored the resonance line [14,15]; subsequent predictions suggested that one of the intercombination lines dominates [16]. Other models, including the most recent one that is based on unresolved laboratory data [17,18], predict the forbidden line to dominate by a wide margin ($\geq 6:1$) over any of the other lines [19,20]. Not surprisingly, laboratory measurements have only recently answered the question whether charge exchange can indeed explain cometary x-ray emission [21]; whether it is a dominant factor in the other nonterrestrial sources of x radiation is still an open question.

Optical emission from charge exchange has been studied on tokamaks and developed into valuable diagnostics [22–25]. Charge exchange with low-energy neutrals is also known to produce x rays in tokamaks [26,27]. In the x-ray regime, it competes, however, with electron-impact excitation, and the contribution from charge exchange to an observed x-ray spectrum has been difficult to isolate in a hot plasma environment. Here we present the K -shell emission spectrum from heliumlike Ar^{16+} recorded at the National

Spherical Torus Experiment (NSTX) that is exclusively excited by an 80 keV neutral deuterium beam in the reaction $\text{Ar}^{17+} + \text{D} \rightarrow \text{Ar}^{16+*} + \text{D}^+$. Using the NSTX high-resolution crystal spectrometer [28] we fully resolved the four K -shell emission lines, allowing us to measure the intensities of the resonance, intercombination, and forbidden lines, enabling a clean test of modeling calculations. In order to predict the emission spectrum produced by charge exchange, we developed an unapproximated radiative cascade model coupled with charge-exchange cross sections obtained using the classical trajectory Monte Carlo (CTMC) approach [29]. Excellent agreement with the experimental data validates our approach and enables us to predict the emission in other spectral ranges.

NSTX plasmas, heated with 2.6 MW of high-harmonic fast-wave radio-frequency (rf) heating power, reach temperatures well above 3 keV [28]. This is enough to produce a substantial fraction of hydrogenlike Ar^{17+} in the plasma center. An 80 keV hydrogen neutral beam may be used to provide additional heating or for probing the plasma. After dissociation, the nominal fractional energy components injected into the plasma are 53% full energy (or 40 keV/amu for deuterium atoms), 32% half energy (20 keV/amu), and 15% third energy (13.3 keV/amu). There is a small fraction of deuterium atoms injected at 4.2 keV/amu following the acceleration and dissociations of deuterated water ions. For the present experiments (shot number 105830), rf heating was turned on from $t=100$ to 300 ms during the discharge. The neutral beam was turned on at $t=220$ ms for a duration of only 20 ms at a power level of 1.5 MW.

The NSTX high-resolution crystal spectrometer views the plasma center through a radial sight line along the midplane of the torus intersecting the neutral beam so that excitation by charge exchange with the neutral beam can be seen with the instrument. The spectrometer focuses on the argon K -shell emission and infers the central ion temperature from the amount of Doppler broadening. The time integration per spectrum is 10 ms. This allowed us to observe the emission before, during, and after the neutral-beam injection, as illustrated in Fig. 1.

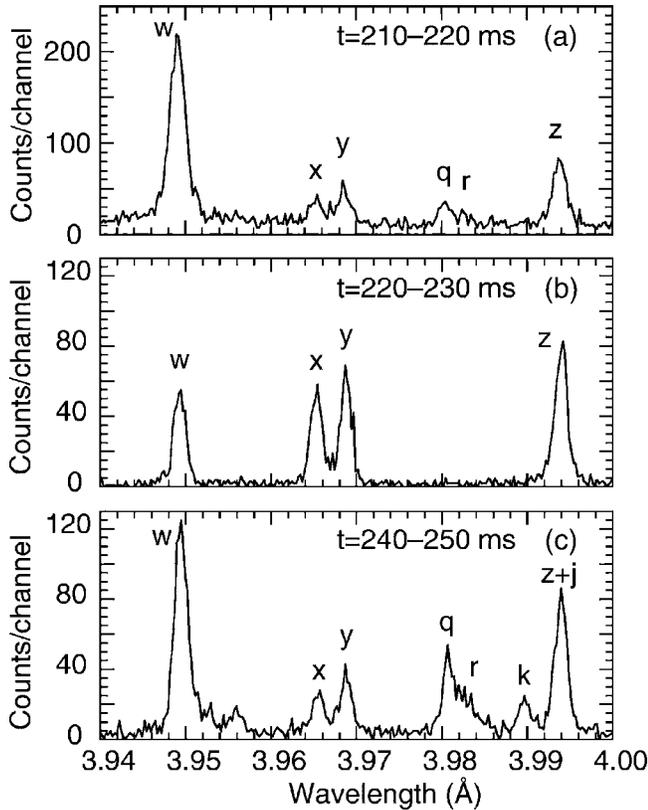


FIG. 1. Spectra of the K -shell emission of argon obtained (a) before, (b) during, and (c) after neutral-beam injection. The integration time for each spectrum is 10 ms. Beam injection commences at $t=220$ and ends at 240 ms.

Before and after neutral-beam injection, the spectrum is typical for electron-impact excitation. The heliumlike resonance line w ($1s2p\ ^1P_1 \rightarrow 1s^2\ ^1S_0$) dominates the spectrum. The two intercombination lines x and y ($1s2p\ ^3P_2 \rightarrow 1s^2\ ^1S_0$ and $1s2p\ ^3P_1 \rightarrow 1s^2\ ^1S_0$, respectively), and the forbidden line z ($1s2s\ ^3S_1 \rightarrow 1s^2\ ^1S_0$) are weak. Also seen are the inner-shell-excited satellite lines q ($1s2s2p\ ^2P_{3/2} \rightarrow 1s^22s\ ^2S_{1/2}$) and r ($1s2s2p\ ^2P_{1/2} \rightarrow 1s^22s\ ^2S_{1/2}$), and the Ar^{15+} dielectronic satellite lines k ($1s2p^2\ ^2D_{3/2} \rightarrow 1s^22p\ ^2P_{1/2}$) and j ($1s2p^2\ ^2D_{5/2} \rightarrow 1s^22p\ ^2P_{3/2}$), whereby the latter line blends with line z .

During neutral-beam injection, the spectrum is dramatically different, showing only the heliumlike lines w , x , y , and z . The reason is that the production of K -shell x-ray emission lines requires a K -shell vacancy. Unlike electron-impact excitation or dielectronic recombination, charge exchange cannot create a K -shell vacancy on its own. It must rely on a preexisting K -shell vacancy in Ar^{17+} in order to produce the x-ray lines w , x , y , and z . Because there is no K -shell vacancy in Ar^{16+} , production of Ar^{15+} x-ray lines by charge exchange is not possible, and lines from Ar^{15+} are not seen. The fact that the K -shell lines from four Ar^{16+} lines are the only lines seen in the spectrum during neutral-beam injection shows that charge exchange is essentially the sole excitation process, and electron-impact excitation of Ar^{16+} and Ar^{15+} has ceased to be relevant. Indeed, the time history of the electron temperature for shot 105830 shows a sudden de-

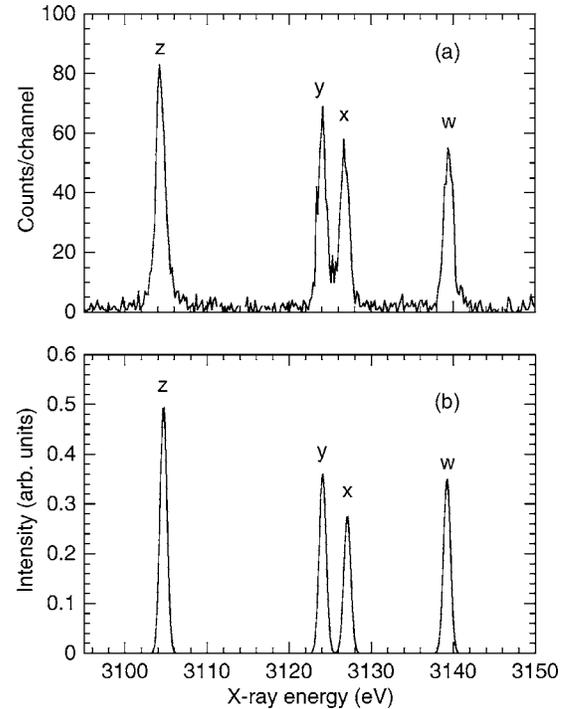


FIG. 2. Spectrum of Ar^{16+} excited by charge exchange between Ar^{17+} ions and a 40 keV/amu neutral hydrogen beam: (a) spectrum recorded on the NSTX tokamak; (b) spectrum predicted by the CHES model. The labels w , x , y , and z denote the resonance, intercombination, and forbidden transitions from upper levels $1s2p\ ^1P_1$, $1s2p\ ^3P_2$, $1s2p\ ^3P_1$, and $1s2s\ ^3S_1$, respectively. The vertical scale in (b) is the same as that in Fig. 3, where unity equals the intensity of the strongest line.

crease of the electron temperature from 3.8 to 0.4 keV at the time of the neutral-beam injection. Details of the experimental conditions of this shot can be found in Ref. [28]. Whether this dramatic drop of the electron temperature was solely caused by the neutral-beam injection or by a magneto hydrodynamic event (internal disruption) that occurred at the same time is not clear. In any case, the—perhaps special—experimental conditions of shot 105830 have allowed us to record a spectrum that is solely produced by charge exchange and in the absence of electron-impact excitation.

Toward the end of and after neutral-beam injection, the spectrum is dominated by lines produced by collisional excitation again. However, the ionization balance is reduced, as indicated by the prominence of the Ar^{15+} line q . The reduction in the ionization balance is expected from the fact that charge exchange is a recombination process and thus has a cooling effect on the heavy trace ions in the plasma. In fact, charge exchange exhausts the reservoir of Ar^{17+} ions so that the charge-exchange-produced emission drops off well before the end of neutral-beam injection.

The intensity of the four heliumlike lines produced by charge exchange is strikingly different from the emission during the electron-impact excitation phase. Line w is no longer the dominant line, as seen from the spectrum in Fig. 2. In fact, it is smaller than either intercombination line. The strongest line is the forbidden line. The dominance of line z is, however, by far not as overwhelming (by factors of 6 or

more) as expected from earlier predictions [19] or from recent models involving lower-*Z* ions [20].

To reproduce the observed x-ray emission we constructed the charge-exchange spectral synthesizer (CHESS) model. The CHESS model employs a detailed radiative cascade matrix. All 1681 levels of the type $1sn\ell$ with $n < 30$ and $\ell < 29$ and all 204 718 electric- and magnetic-dipole and quadrupole transitions between them were calculated using the flexible atomic code [30] and included in the CHESS model. Two-photon decay, which is the dominant decay path for the $1s2s^1S_0$ level, was also included by employing the rates calculated by Lin, Johnson, and Dalgarno [31]. Line emission was calculated by following all radiative decay paths starting from the initial level population. The latter is given by the CTMC calculations [32,33], which yield charge-exchange cross sections that are resolved by the principal quantum number n and angular quantum number ℓ . Singlet and triplet states are populated statistically. Our calculations show that only 1% of the total charge-exchange recombination cross section in a 40 keV/amu collision populates levels with principal quantum number $n=17$ or higher. The fraction is even less for the lower collision energies, which justifies limiting our atomic cascade model to $n < 30$. The cross section peaks for capture into $n=9, 10$.

The CHESS results are shown in Fig. 2(b) for comparison with the experimental data. We calculated charge-exchange cross sections for all four constituent energy fractions in our deuterium beam. Although the cross sections themselves vary in energy, no significant differences are found in the computed x-ray emission spectra, as illustrated in Fig. 3. A dependence of the spectral emission of hydrogenic ions on the collision energy had been noted earlier [33,34], but this dependence sets in mainly for energies below about 1 keV/amu, i.e., at energies where the population of different angular momentum states differs significantly from that expected from statistics.

The agreement of the model spectrum with the measurement is very good. The model correctly predicts the dominance of the forbidden and intercombination lines, although it slightly underestimates the intensity of line *x* at the expense of line *w*. We stress that the CHESS model is a fully *ab initio* model; no adjustments based on empirical results have been made except for the values of the transition energies.

The success of our model encourages its use for predictions in other spectral regions. Such predictions are automatically produced by the CHESS model, as it incorporates the full atomic structure. Results are shown in Fig. 4 for photon energies between 0 and 600 eV. These results should be testable in future experiments on tokamaks viewing the soft x-ray and the extreme ultraviolet region.

We note that the spectral emission may be affected by charge exchange with hydrogen in the $2s$ metastable state, as pointed out by Rice *et al.* [27]. A typical estimate is that about 0.5% of the hydrogen in a neutral beam is in this metastable configuration [35]. Although the typical cross section for charge exchange with metastable hydrogen is about an order of magnitude larger than that for charge exchange with ground-state hydrogen, any correction will be relatively minor. CHESS calculations for collisions solely

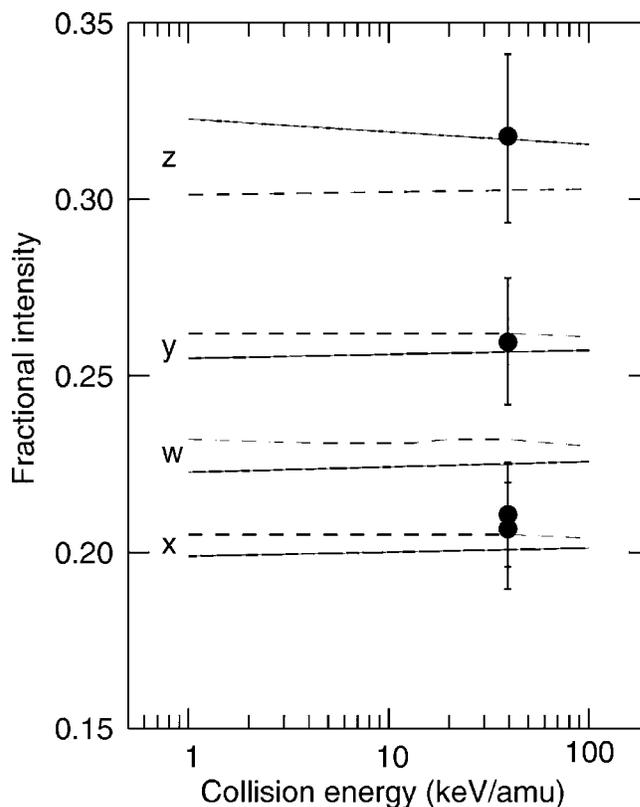


FIG. 3. Comparison of the measured fractional Ar^{16+} line intensities with those predicted by the CHESS model for charge exchange with hydrogen in the ground state (solid line) and hydrogen in the $2s$ metastable state (dashed line).

with hydrogen in the $2s$ metastable state show a small departure of the fractional intensities of the four Ar^{16+} lines from those calculated for collisions with hydrogen in the ground state. Mainly, the fractional intensity of the forbidden line decreases at the expense of all other three lines, as shown in Fig. 3. The differences between the two calculations are less than the uncertainties of the measurement.

In summary, we have presented a fine-structure-resolved x-ray emission spectrum excited solely by charge exchange. A clear signature of the excitation by charge exchange is seen. While the singlet line is the dominant transition in collisional plasmas, our measurements reveal it to be the weakest, albeit comparable with *x*. All three triplet lines are stron-

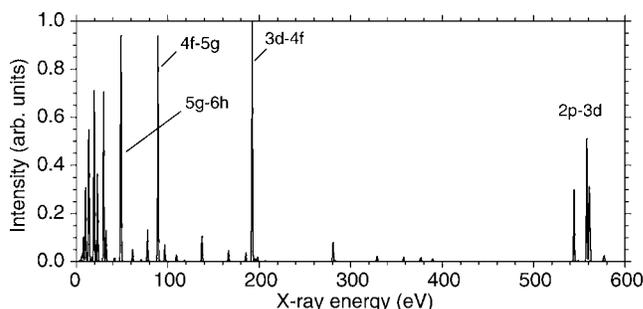


FIG. 4. Spectral line emission of Ar^{16+} below 600 eV induced by charge exchange between Ar^{17+} ions and a 40 keV/amu neutral hydrogen beam predicted by the CHESS model.

ger and their combined sum is about four times the intensity of the singlet line. A fully *ab initio* charge-exchange spectral synthesizer model was presented that includes all atomic levels, all allowed and dipole- and quadrupole-forbidden transitions, and charge-exchange cross sections calculated by the CTMC method. Unlike earlier predictions of the *K*-shell x-ray emission, the model yields very good agreement with the observations, validating our model and the applicability of the CTMC approach for calculating charge exchange cross sections in the present energy regime. The modeling calculations allow us to make predictions in other spectral bands, in particular of the *L*-shell emission, which provides the bulk

of the soft x-ray flux from comets and planetary atmospheres.

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