Charge Dependence of Total K-Shell Vacancy-Production Cross Sections in Argon by the Impact of Heavy Ions

J. H. McGuire
Department of Physics, Kansas State University, Manhattan, Kansas 66506
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The charge dependence of K-shell-electron vacancy production in argon by heavy-ion impact is found by adding charge-exchange and ionization cross sections computed in the binary-encounter approximation. The dependence of these cross sections on the nuclear charge, for fully stripped ions ($z=6$, 7, 8, and 9), is in agreement with recent experimental results at 1.88 MeV/amu, where large deviations (>100%) from a z^2 dependence were observed. The dependence of atomic charge q for F^{+q} at 1.88 MeV/amu ($q=9$, 7, 8, 6, and 5) is in reasonable agreement with experiment.

Quite recently there have been two types of observations[1,2] of the dependence of K-shell x-ray yields in argon on projectile charge. In the first,[1] the Ar x-ray yield was measured as a function of the atomic charge q for fluorine ions F^{+q} ($q=9$, 8, 7, 6, and 5). The cross section observed for the fully stripped ion at 35.7 MeV is a factor of 3 above the theoretical ionization cross section computed in either the Born[3] or classical binary-encounter[4-7] approximation. Furthermore, the observed cross sections decreased rapidly as electrons were added to the fluorine ion and could not be fitted with a q^2 dependence. In the second[2] experiment, the cross section was measured as a function of the nuclear projectile charge z for fully stripped ions ($z=1$, 6, 7, 8, and 9) near 1.88 MeV/amu. In this case, the large deviation from the z^2 dependence predicted by the Born and binary-encounter models cannot be fitted with a binding-energy correction,[8] an initial-state polarization correction,[8,9] or a final-state polarization correction.[10] Nor does it seem likely that z-dependent corrections in the Glauber approximation[11] will work. In this paper both the atomic- and nuclear-charge dependence are explained by interpreting the total K-shell vacancy-production cross sections as the sum of ionization[12] and charge-transfer[12,13] cross sections.

The classical binary-encounter model has been used to compute ionization and charge-transfer cross sections by trivially extending the results of Garcia, Gerjuoy, and Welker for ionization[7] and charge exchange[12] with proton beams. In their model, the two-body Coulomb cross section between the projectile p and the participating atomic electron e is computed as a function of energy transfer ΔE, namely,

$$\sigma(v_p, v_e) = \int \frac{d\sigma(v_p, v_e, \Delta E)}{d\Delta E} d\Delta E .$$

This two-body cross section is then integrated over a hydrogenic electron density distribution in the standard way.[7,12] The sole difference in the computations for ionization and charge transfer is the range of energy transfers used: For ionization,[4,7] $U_T \leq \Delta E \leq E_p$, and for charge exchange,[4,12] $\frac{1}{2}M_e v_p^2 + U_T - U_p \leq \Delta E \leq \frac{1}{2}M_e v_p^2 + U_T + U_p$, where $U_{T(p)}$ is the target (projectile) binding energy, $E_p(v_p)$ the projectile energy (velocity), and M_e the electron mass. For protons with energies

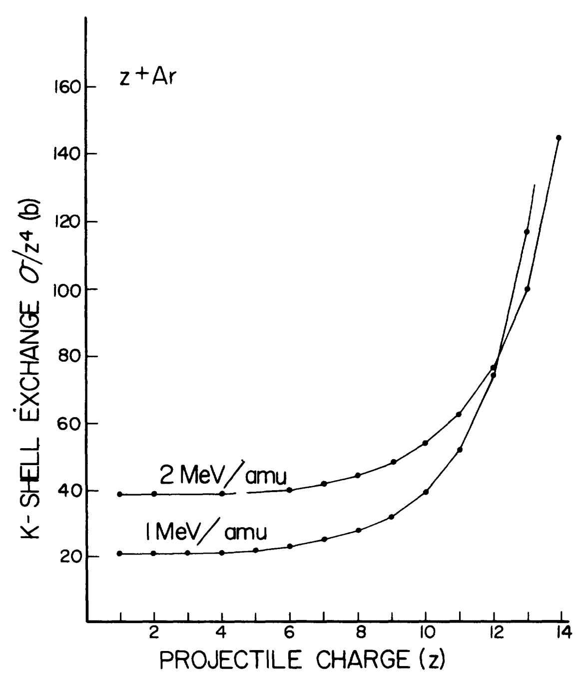

FIG. 1. Charge-exchange cross section from the K shell of Ar to the $N=1$ level of a particle projectile with charge z, divided by z^4. The cross section to all levels of the projectile is ~1.64 times as large as the values shown for $z<10$.

above 10 keV, predictions based on this model are within a factor of 2 of experiment for total-charge exchange[12] and ionization[7] in argon.

Unfortunately, both the Born[13] and binary-encounter[12,14] calculations overestimate charge-exchange cross sections for outer-shell phenomena when the projectile velocity is less than the velocity of the orbiting atomic electron. Hence, application of the binary-encounter model to inner-shell exchange phenomena at the edge of the low-velocity region should be regarded with caution, and predictions at lower velocities regarded with outright suspicion. Furthermore, in the classical binary-encounter model, cross sections rather than amplitudes are added; there is no rigorous justification. However, the technique works reasonably well in the continuum, so that an extension at least into the higher-lying quantum levels seems plausible, especially since the Born calculations, which include interference effects, give qualitatively the same results.

Cross sections for charge exchange from the K shell of Ar to the projectile K shell are shown in Fig. 1 as a function of nuclear fully stripped projectile charge z at 1 and 2 MeV/amu. For small z, corresponding[12] to $U_P < U_T$, the exchange cross section is proportional to z^4 and N^{-2}, where N denotes the electronic level in the projectile. Hence, the cross section for exchange to all levels

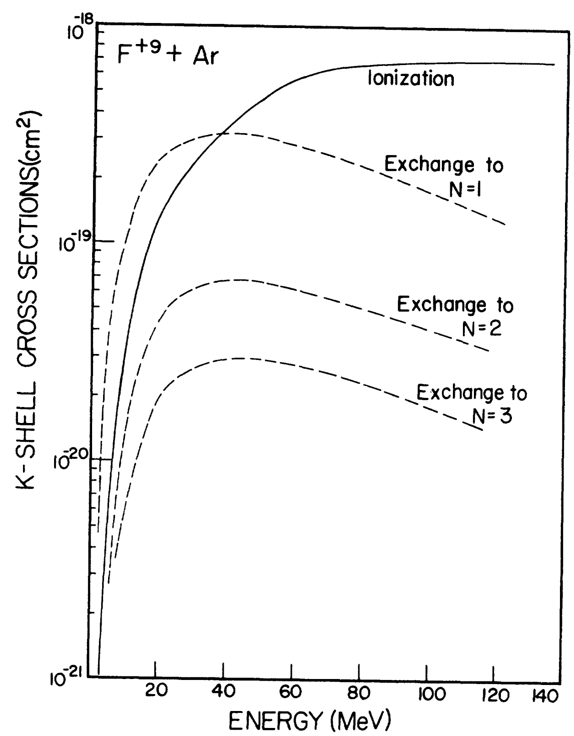

FIG. 3. Ionization and charge-exchange cross sections vs energy for F^{+9}+Ar. These Ar K-shell cross sections approximately scale as N^{-2}, where N denotes the electron level in F. At the lower energies, the charge-exchange predictions may be too large (cf. Ref. 12).

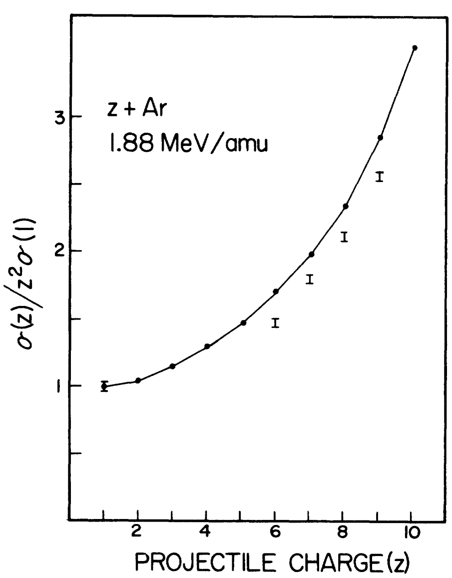

FIG. 2. Total K-shell cross-section ratio vs projectile charge at 1.88 MeV. The total cross section is the sum of the ionization and charge-exchange cross sections. Data at z = 6, 7, 8, and 9 for fully stripped heavy ions are from Macdonald *et al.* (Ref. 2). The experimental cross section for protons is 3.3×10^{-21} cm^2, in agreement with the computed value of 3.36×10^{-21} cm^2.

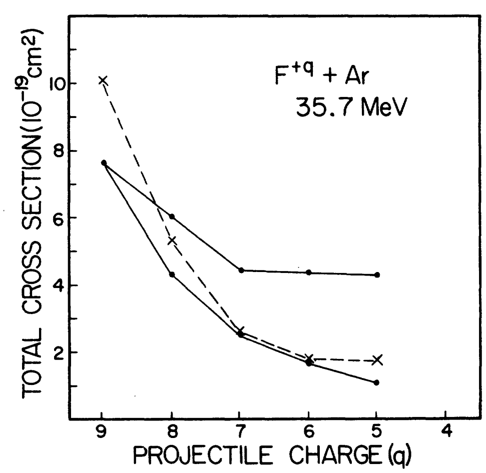

FIG. 4. Dependence of the total cross section of projectile charge. The upper solid curve represents calculations using the nuclear charge (+9) of F, the lower solid curve represents calculations using the atomic charge (+q) of F, and the dashed curve represents the date of Macdonald *et al.* (Ref. 1). In both calculations, the charge-exchange cross sections are statistically reduced according to the number of projectile vacancies available.

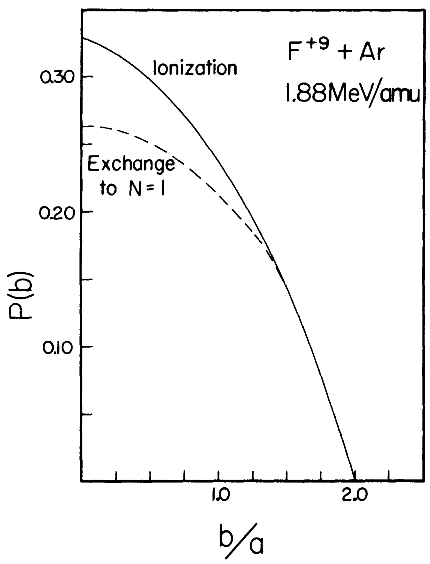

FIG. 5. Probability vs impact parameter. The impact parameter b is measured in units of atomic K-shell radius a.

is a factor of $\sum_{N=1}^{\infty} N^{-2} = \frac{1}{6}\pi^2$ larger than exchange to the $N = 1$ level.

The dependence of the total Ar K-shell cross section (exchange to all projectile levels plus ionization) on fully stripped projectile charge is shown in Fig. 2. The results are in agreement with the recent results of Macdonald[2] *et al.*

Individual K-shell exchange and ionization cross sections are plotted as a function of energy for a F^{+9} projectile in Fig. 3. At low energies the exchange cross section is seen to dominate, owing to a difference in the energy dependence of the charge-exchange and ionization cross sections.

In Fig. 4, the total cross section is plotted as a function of atomic charge q for 35.7-MeV F^{+q} on Ar and compared with experiment.[1] Since the exchange and ionization probabilities (Fig. 5) are large over a distance comparable to the radius of K-shell electrons in fluorine, it is difficult to say whether the atomic charge q or the nuclear charge z should be used in computing cross sections. Consequently, two calculations were done. In the first, the screening effects of the projectile electrons were ignored (i.e., the nuclear charge z was used). Since the $q = 7$ state of fluorine has a filled K shell, charge exchange to the $N = 1$ level of F^{+7} was set equal to zero. Similarly, charge exchange to the $N = 2$ levels was statistically reduced according to the number of vacancies available. In the second calculation, the effect of filling projectile levels was treated in the same fashion, but the atomic charge q was used in place of the nuclear charge z. Using the two extreme screening approximations for the effective projectile charge tends to bracket the experimental results. For fully stripped F^{+9} ions the ionization cross section is 3.37×10^{-19} cm^2 and the total exchange cross section is 4.30×10^{-19} cm^2.

Similar calculations have been compared to experiment[15] for F^{+q} + Ar at 1.58 and 1.05 MeV/amu and for Si^{+12} + Ar using the atomic charge q. The calculations are within 50% of experiment at all points, overestimating the data at lower energies.

While the quantitative agreement of present calculations with experiment is probably fortitious owing to the limitations of the calculations, I conclude that for highly charged heavy ions, exchange cross sections for inner-shell electrons are not always small compared to the ionization cross sections. The clear experimental data now available provide strong incentive for more thorough calculations of atomic vacancy production, including both Coulomb ionization and charge transfer.

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