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K-shell ionization of light elements by proton and helium-3–ion impact

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K-shell ionization cross sections for Al and Si by proton and ^{3}He-ion impacts have been measured with thin targets and a proportional counter over the projectile energy range 0.75–4 MeV/amu. The results, together with others on light elements, are compared with theoretical predictions based on the plane-wave Born approximation and the binary-encounter approximation, and it is found that the scaling law, taking into account the effects of the Coulomb deflection of the projectile and the increase of binding energy of *K*-shell electrons, gives a good fit to the experimental results over the entire energy range measured. Ratios of the *K*-shell ionization cross sections for helium-ion impact to those for proton impact show deviations from the Z_1^2 dependence predicted by the Coulomb interaction theory. Possible reasons for this deviation are discussed.

I. INTRODUCTION

A number of data on *K*-shell ionization by heavy-charged-particle impact for light elements ($Z_2 \leqslant 20$, Z_2 being the nuclear charge of the target) have been obtained, especially at lower velocities ($v_1/v_0 < 1$, where v_1 and v_0 are the velocities of the projectile and of *K*-shell electron, respectively).[1] Data are still limited at higher energies ($v_1/v_0 > 1$), where theoretical calculations based on the Born approximation would be more reliable. Most of these data are based on x-ray measurements from thick targets. In such measurements, there are some problems concerned with the stopping power of target material for the projectile and with the x-ray absorption in the target, which are not always accurately known. Therefore these data usually contain large errors, typically 30–50%. Furthermore, the fluorescence yields for these low-*Z* elements are very small and are not accurately known.[2] For the investigation of inner-shell ionization for very-low-*Z* elements, measurements of the Auger electron are preferable to x-ray measurements. However, the former can be applied only to gaseous targets, while the latter can be applied to any target.

Recently some accurate calculations[3] of the fluorescence yield have been performed and were found to agree rather well with available data. In this paper we report the results on Al and Si *K*-shell ionization in proton and helium-3-ion impact where thin targets were used in order to avoid the problems in thick-target measurements mentioned above (see Fig. 1). The scaling law on *K*-shell ionization for light elements is also discussed, based on available theories.[4,5] Furthermore, remarkable deviations of experimental data from the Coulomb interaction theory in helium-ion impact are discussed.

II. THEORIES

For describing *K*-shell ionization by ion impact, two theories are generally used, namely, the plane-wave Born approximation (PWBA) and the binary-encounter approximation (BEA).

A. PWBA

The PWBA is discussed in detail by Merzbacher and Lewis[4] and by Basbas *et al.*[6] The *K*-shell ionization cross section is given by

$$\sigma_{Ki}^{\mathrm{PWBA}} = (\sigma_{0K}/\theta_K)F(\eta_K/\theta_K^2)\,, \tag{1}$$

where

$$\sigma_{0K} = 8\pi(Z_1/Z_{2K}^2)^2 a_0^2, \quad \theta_K = U_K/Z_{2K}^2\mathcal{R}\,,$$

$$\eta_K = Z_{2K}^2\mathcal{R}(m/M)E_1, \quad Z_{2K} = Z_2 - 0.3\,,$$

and where Z_1 and Z_2 are the nuclear charges of the projectile and target, respectively; E_1 is the incident energy of the projectile, U_K is the binding energy of *K*-shell electrons, $\mathcal{R}$ is the Rydberg constant, m and M are the masses of an electron and the projectile, a_0 is the Bohr radius, and F is a universal function of η_K/θ_K^2 given by Basbas *et al.*[6] This cross section is plotted in Fig. 2; the curve is considerably higher than the experimental data at lower energies. Basbas *et al.*[6] introduced corrections due to the Coulomb deflection of the projectile and the increased binding energy of *K*-shell electrons in order to improve the agreement between the PWBA and experiment. The PWBA with these corrections gives the cross section as

$$\sigma_{Ki}^{\mathrm{PWBA}} = 9E_{10}(a\epsilon\,\theta_K\eta_K^{-3/2})(\sigma_{0K}/\epsilon\,\theta_K)F(\eta_K/(\epsilon\theta_K)^2)\,. \tag{2}$$

Here a is a constant, E_{10} is the exponential integral of order 10, and ϵ is the correction factor

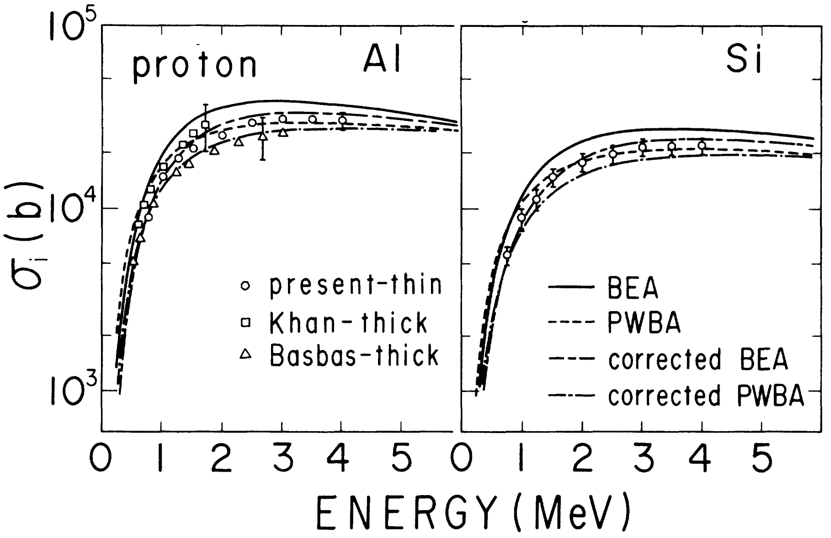

FIG. 1. K-shell ionization cross sections for proton impact on Al and Si, together with other experimental results obtained using thick targets and the theoretical predictions, where "corrected" means the corrections for the increased binding energy and the Coulomb deflection of the projectile.

for the increased binding energy. The first term of the right-hand side denotes the correction due to the Coulomb deflection of the projectile. The binding-energy correction is given simply by changing θ_K to $\epsilon\theta_K$ ($\epsilon \geq 1$) in Eq. (1). This curve is also universal and is shown in Fig. 3.

B. BEA

The BEA was introduced by Garcia,[5] and the K-shell ionization cross section is given as follows:

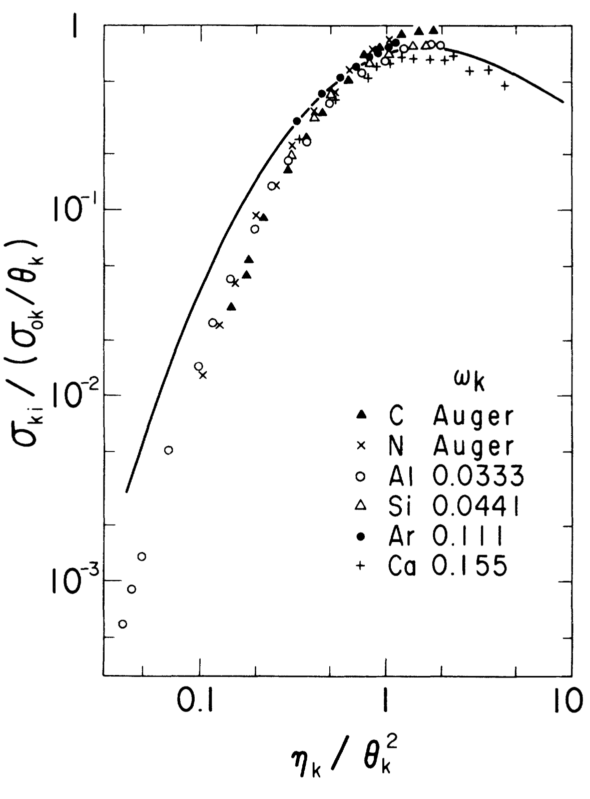

FIG. 2. Comparison of the K-shell ionization cross sections for light elements with the scaled universal PWBA curve without any correction.

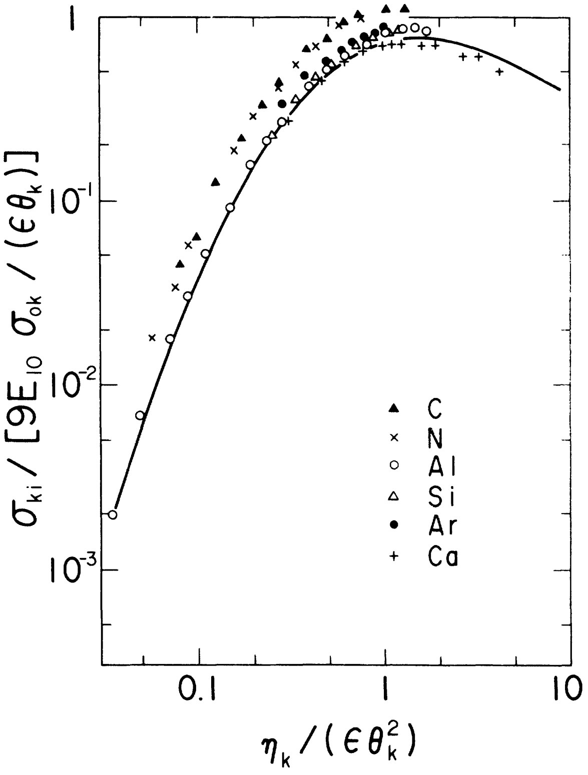

FIG. 3. Comparison of the K-shell ionization cross sections with the scaled PWBA curve with corrections for the increased binding energy and the Coulomb deflection of the projectile.

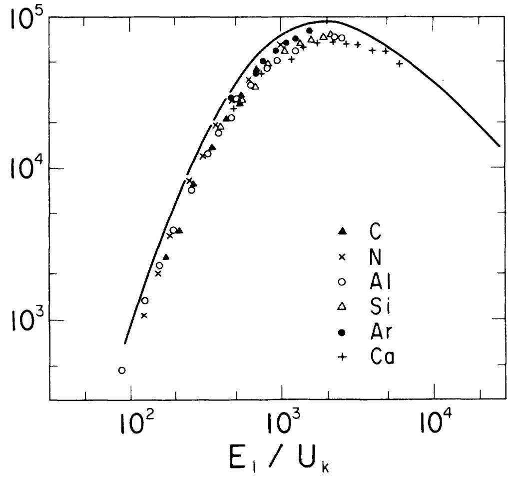

FIG. 4. Comparison of the K-shell ionization cross sections with the universal BEA curve without any correction.

$$\sigma_{Ki}^{\mathrm{BEA}} = (Z_1^2/U_K^2)G(E_1/U_K)\,. \qquad (3)$$

Here G is a universal function depending only on E_1/U_K. This is given in Fig. 4. The binding-energy effect can also be incorporated with the BEA by substituting U_K in Eq. (3) with ϵU_K. The effects of the Coulomb deflection and the reduction of the kinetic energy of the projectile were estimated by Garcia and, for the present energy region, these corrections are only a few percent and are neglected here (see the curve in Fig. 5).

As discussed, the important point in the PWBA and the BEA is the fact that K-shell ionization cross sections can be expressed by the scaling law for various elements and various projectiles.

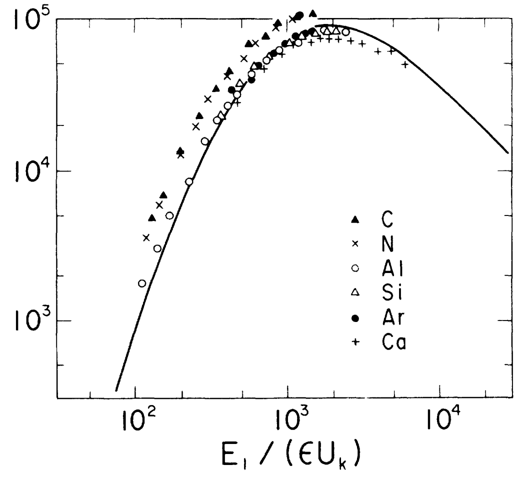

FIG. 5. Comparison of the K-shell ionization cross sections with the BEA curve with corrections for the increased binding energy and the Coulomb deflection.

III. EXPERIMENT

The experimental setup for the present measurements has already been given in detail elsewhere (see Ref. 15). Only the description relevant to the present experiment is given here. Thin self-supported Al and Si targets (~ 100 μg/cm^2) were prepared by vacuum evaporation and positioned at 45° to the beam direction. A flow-mode proportional counter with a 6-μm Mylar window was used to detect these soft x rays. The detection efficiency of the counter was determined experimentally via standard techniques, i.e., by putting the second foil in front of the first foil and by changing the gas pressure of the counter. The uncertainties in the present data are estimated to be about 12%, originating mainly from those in the target thickness which were determined from Rutherford scattering of helium ions.

To convert the measured x-ray production cross section to the ionization cross section, the calculated fluorescence yields ($\omega_K = 0.0333$ for Al and 0.0441 for Si) of Kostroun *et al.*[3] listed by Bambyneck *et al.*[2] were used.

IV. PROTON IMPACT

A. Experimental results and comparison with theory

The present K-shell x-ray production cross sections are listed in Table I and are shown in Fig. 1 for Al and Si along with various theoretical predictions; they are also compared with previous data of Khan *et al.*[7] and Basbas *et al.*,[6] both of whom used thick targets. Typical error bars for each measurement are shown in the figure. Errors in the present data are about one-third of those in the previous data.

Generally, the PWBA without any correction for the binding-energy and the Coulomb deflection effects can better reproduce the experimental data,

TABLE I. K-shell x-ray production cross sections of Al and Si in proton and ^{3}He-ion impact in units of 10^{-22} cm^2.

Energy	Al		Si	
(MeV/amu)	H	^{3}He	H	^{3}He
0.75	2.96	8.08	2.47	6.28
1.00	4.78	14.5	3.95	11.5
1.25	6.16	20.8	4.85	16.7
1.50	6.98	26.6	6.35	22.7
2.00	8.10	36.8	7.68	32.0
2.50	9.47	43.5	8.61	36.8
3.00	9.93	46.5	9.34	39.1
3.50	9.98	···	9.55	···
4.00	9.73	···	9.60	···

except at low energies where the PWBA with these corrections gives a nice fit to the observed results. In the present energy region, the correction for the increased binding energy is dominant compared with that for the Coulomb deflection. On the other hand, the BEA predicts values considerably higher than the measurements. However, the BEA with these corrections comes close to the experimental data over the whole energy range investigated.

B. Scaling laws

In order to test the scaling laws from the PWBA and the BEA discussed in Sec. II, we show in Figs. 2-5 in universal forms, a number of data on the K-shell ionization for light elements ($Z \leq 20$) taken from various sources.[8-10] For consistency, the fluorescence yields of Kostroun *et al.*[3] are used for all elements shown except C and N, where the Auger electrons were measured instead of x rays.

The curve in Fig. 2 shows the PWBA without any correction [Eq. (1)] in the universal fit described by Basbas *et al.*[6] At lower energies, the PWBA predicts considerably higher values. It should be noted, however, that the experimental data fall almost on a single curve. Figure 3 shows the experimental data and the scaled PWBA curve with the corrections for the increased binding energy and the Coulomb deflection in a form discussed by Basbas *et al.*[6] [Eq. (2)]. From this figure it is clear that all of the observed data come close to the PWBA with the corrections over the whole energy range, except those for C and N which are considerably higher than the PWBA. On the other hand, the BEA universal curve without any correction is systematically higher than experimental data (see Fig. 4). As shown in Fig. 5, the BEA with corrections again comes close to the experimental values over the whole energy range, except for the C and N data.

It may be guessed that similar discrepancies found for C and N between experiment and the predictions of the PWBA and BEA with corrections mean that the correction of the binding-energy effect is overestimated for these very light elements, although there are some inherent uncertainties connected with the fluorescence yield in the x-ray measurements.

V. ^{3}He ION IMPACT

In Table I are shown the measured x-ray production cross sections for ^{3}He-ion impact, which were determined relative to those in 3-MeV proton impact. There are some other data measured for Al by Sellers *et al.*,[11] who used a thin target and α particles from ^{241}Am, and by Basbas *et al.*,[6]

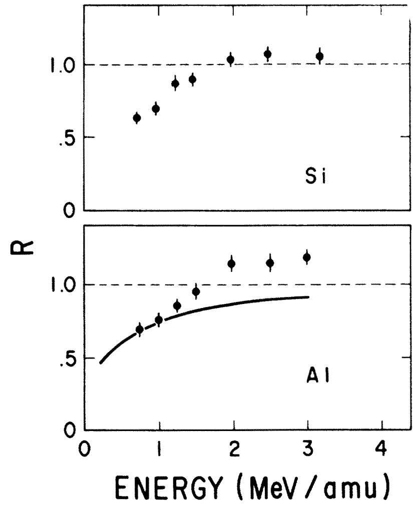

FIG. 6. Ratio R of the K-shell ionization cross sections for helium-ion impact to those for proton impact divided by 4 as a function of the projectile energy (MeV/amu). The solid curve shows the prediction by Basbas *et al.* taking into account the effect of the increased binding energy.

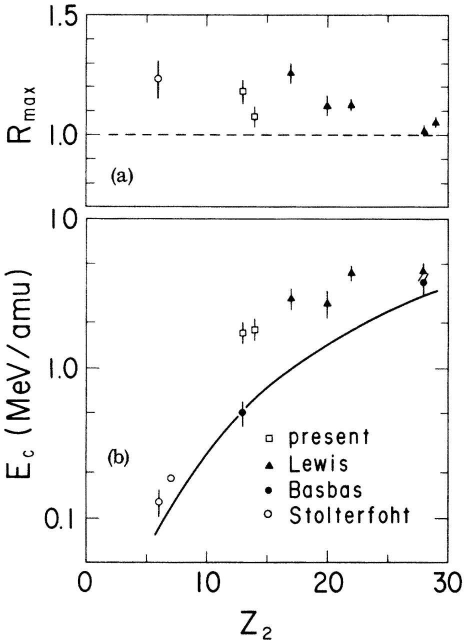

FIG. 7. (a) Upper figure shows the maximum value of R vs the target nuclear charge Z_2, together with other experimental results. (b) Lower figure shows the energy for the crossing point of $R = 1$, together with those from experiment. The solid curve shows that derived by Basbas *et al.* taking into account the effects of increased binding energy and the polarization of orbit.

who used a thick target. Surprisingly, there are large discrepancies between the present data and those of Sellers *et al.*, on the order of a factor of 2 in the overlapped energy range. Those of Basbas *et al.* are between those of Sellers *et al.* and of this work and tend to approach the present data at higher energies. It is conjectured that those of Sellers *et al.* are too high (see discussion below).

Instead of comparing the data on helium impact with theory we compare values of $R = \sigma_{Ki}(\mathrm{He})/4\sigma_{Ki}(\mathrm{H})$, where $\sigma_{Ki}(\mathrm{H})$ and $\sigma_{Ki}(\mathrm{He})$ are the K-shell ionization cross sections by proton and ^{3}He-ion impact, respectively, since this is a more rigorous test of the discrepancy between experiment and theory. As shown by Basbas *et al.*[6] and Lewis *et al.*,[12] the ratios R are smaller than unity at low energies and become larger than unity at high energies. Than at much higher energies, R approaches unity as expected from the Coulomb interaction theory. Thus R becomes unity at an intermediate energy which we call the corssing point.

In Fig. 6 are shown values of R taken from the present measurements on Al and Si targets. The maximum values of R, shown in Fig. 7(a) together with other experimental results, are usually 1.05–1.3 for targets of light elements ($6 \leq Z \leq 22$). The present data are consistent with other data. However, if those of Sellers *et al.* were used, the maximum value of R for Al would be about 2.4, which is too high compared with other data. The observed crossing points, where R is unity, are shown in Fig. 7(b) for Al and Si targets, together with those for some other elements.[12-14] The solid curve shows the expected crossing points for K-shell ionization discussed by Basbas *et al.*,[13] and is given as follows[15]:

$$E_c = 1.83U_K(U_K/2\mathcal{R}Z_{2K}^2)^2\,, \qquad (4)$$

where U_K is the binding energy of the K-shell electrons, $\mathcal{R}$ is the Rydberg constant, and Z_{2K} is the effective nuclear charge ($=Z_2 - 0.3$). The experimental data points are always higher than the values predicted by Basbas *et al.* except for their own data on Al. If the data of Sellers *et al.* on helium-ion impact were used, the crossing point Al would be about 300 keV, which is considerably lower than the prediction and again far from the general trend observed so far.

VI. DISCUSSION

It is found in the present measurement that the K-shell ionization cross sections for light elements by proton impact can be reproduced fairly well with the PWBA with corrections for the Coulomb deflection and the increased binding energy at energies lower than ~1.5 MeV and with the PWBA without any correction at higher energies. The BEA predicts somewhat higher values over the whole energy range studied, but the BEA with the corrections reproduces the observed data well. If the corrections for the Coulomb deflection and the binding-energy effect are applied, the scaling laws based on the PWBA and the BEA hold quite well for low-Z elements except for C and N. It is conjectured that the correction for the binding-energy effect is overestimated for these very-low-Z elements.

However, the ratios R of K-shell ionization cross sections in helium-ion impact to those in proton impact divided by 4 deviate considerably from the theoretical value of unity. A number of possible reasons for the deviation can be considered. As shown by the solid curve in Fig. 6, the deviation in R can be well described by the binding-energy and Coulomb deflection effects at lower energies. However, at higher energies, R becomes larger than unity. Some reasons for this are now discussed.

(a) Polarization of the electron orbit. Basbas *et al.*[13] argued that the polarization of the K-shell orbit due to the proximity of the projectile is responsible for this increased R but did not give details of their analysis for this effect. By taking into account Coulomb deflection increaed binding energy, and polarization of the orbit, they gave the crossing point, as shown by Eq. (4), without detailed discussion. As seen in Fig. 7, the predicted crossing points are considerably lower than the observed values.

(b) Multiple ionization. It is known that owing to multiple ionization, i.e., K-shell ionization accompanied by L-shell ionization, the fluorescence yield of atoms increases considerably. According to the calculation of Bhalla,[16] the fluorescence yields of Al are 0.041, 0.042, 0.044, and 0.045 for K, KL^1, KL^2 and KL^3 configurations, respectively[17] (KL^2, for example, denotes K-shell ionization with two L-shell electron ionizations). On the other hand, probabilities of multiple ionization have been measured in helium ion impact by Richard *et al.*[17] Their results show that probabilities of multiple ionization at 1-MeV/amu impact energy are 0.389, 0.457, 0.135, and 0.019 for the above configurations, respectively. From these values, the increase in the fluorescence yield of Al at 1-MeV/amu helium-ion impact is estimated to be about 2%, compared with that in proton impact where single K-shell ionization is known to be dominant. As the impact energy increases, single K-shell ionization becomes dominant and the probability of multiple ionization decreases. Therefore in the present energy range multiple ionizations cannot be responsible or at

least not be a main cause of, the deviation in R from unity.

(c) Charge transfer to bound states of projectile. The charge transfer of K-shell electrons to the bound states of the projectile becomes noticeable in completely ionized heavy-ion impact. According to discussions of Halpern and Law,[18] the charge transfer cross section for K-shell electrons is estimated to be 5.8×10^{-21} cm^2, which is about 4% of the observed total K-shell ionization at 2.85-MeV/amu helium-ion impact, where the velocity of K-shell electron of Al is equal to that of the projectile; meanwhile, the cross section for proton impact is 1.5×10^{-22} cm^2, only 0.5% of the observed K-shell ionization.[19] Then about 30% of the deviation in R from unity can be due to the charge transfer to the bound states.

(d) Charge transfer to continuum. The charge transfer of K-shell electrons to the continuum of the projectile has been discussed by Doolen *et al.*,[20] who showed that this process becomes important at higher energies where the projectile moves faster than K-shell electrons. The calculation shows that R for Al is about 1.23 at 2.85-MeV/amu impact energy. If this value is combined with the binding-energy and Coulomb deflection corrections of Basbas *et al.*,[6] R is found to be about 1.1, which is reasonably close to the observed value. But at lower energies, the effect is overestimated, resulting in higher values of R compared with the observed data.

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