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BINDING, COULOMB AND RELATIVISTIC EFFECTS IN K-SHELL IONIZATION

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The experimental values of the ionization cross sections and ratios are discussed in the light of theoretical calculations based on the first order Born approximation or (SCA) semi-classical approximation including main corrections at low projectile velocities—Binding (B), Coulomb (C), and Relativistic (R).

It is concluded that the cross sections calculated according to these procedures are in good agreement with the experimental data.

Key Words : Binding; Coulomb; Relativistic; K-Shell; Ionization; Born Approximation; Semi-classical Approximation

Introduction

Inner shell hole production by heavy charged particles has been the subject of many theoretical and experimental refinements in the last few years.[1–6] Detailed theoretical work has been made to account for the binding, Coulomb retardation, relativistic and energy loss effect, thus producing numbers demanding a higher degree of accuracy in their comparison with experiments.

In this paper, our interest is mainly focussed on aspects of the ionization process which are of importance for the total cross sections. From a theoretical point of view, the high Z-targets provide a severe testing ground for the refinements to various models, inasmuch as the simple versions of ionization theory such as the non-relativistic straight line semi-classical approximation (SCA) or the plane wave Born approximation (PWBA) clearly will be insufficient.

To get a reasonable agreement with the experimental cross sections, the relativistic motion of the K-shell electrons in heavy target atoms, the retardation and deflection of the projectile caused by the Coulomb interaction with the target nuclei, and the change in binding energy stemming from the interaction of the electrons with both target and projectile during the collision are to be considered.

Theory

First-order Born Approximation (SCA)

In the impact parameter formulation, first-order Born approximation leads to the expression

$$a_n = - i/\hbar \int_{-\infty}^{\infty} \mathrm{d}t < n \mid V(P, t) \mid 0 > \exp(iwt) \qquad \ldots(1)$$

for the amplitude for a transition of an electron in a bound state $\mid 0 >$ to a final state $| n >$. The transition frequency ω is given by $\omega = (E_n - E_o) | \hbar$. The potential $V(P, t)$ represents the time-dependent interaction between the electron and the projectile moving in a straight-line path at impact parameter P, i.e., with coordinates relative to the centre of the target atom, $R(t) = (P, O, Z = vt)$. Already from formula (1), one may draw some qualitative conclusions about the effective region of interaction. The contribution to the integral from times $| t | > \frac{1}{\omega}$ will tend to cancel by destructive interference, and the effective path length contributing to the amplitude will be of order $\Delta z \sim \frac{V}{\omega}$. This distance, which is usually called the adiabatic distance corresponding to an energy transfer $\Delta E = \hbar \omega$, also determines the range of impact parameters contributing to the total cross section for the transition. In order to see this qualitatively, we consider the expression for the amplitude, which is obtained from equation (1) after some calculations by Bang and Hansteen[7] and Madison and Merzbacher.[8]

$$a_n = 2iz \frac{z}{hv} < n \mid K_0(r_i - P \mid r_{ad}) \exp (iq_0 z) \mid 0 > \qquad ...(2)$$

The symbols r_i and P denote vectors in the x-y plane corresponding to the coordinates of the electron and projectile, respectively while q_0 is defined as $q_0 = \frac{1}{r_{ad}}$, and z values are the coordinates of the electron the function K_0 is modified Bessel which decreases exponentially for large values of the argument. Thus for large values of the impact parameter P relative to the adiabatic distance r_{ad} and to spatial extension of the wave function, the amplitude will decrease exponentially, the ionizing collision becoming increasingly adiabatic. However, since the argument of the K_0 function depends on the impact parameter, relative to the position of the electron, this function cannot alone explain a dependence of the transition probability on P, which is narrower than the spatial extension of the wave function; this is accomplished by the second factor in the matrix element, exp (iq_0^z), which defines the momentum transfer in the z-direction to be

$$\overline{\Delta}_p \cdot (\bar{V}/V) = \hbar q_0, \text{ or } \overline{\Delta}_p \cdot \bar{V} = \hbar\omega = \Delta E, \qquad ...(3)$$

corresponding to the energy momentum relation for an infinitely heavy projectile. At low velocities, this momentum transfer is large compared to the characteristic momentum of the bound electron. For K-shell ionization, one can introduce the parameter ξ,

$$\xi = r_{ad}/r_k = q_k/q_0, \qquad ...(4)$$

where hq_k is characteristic K-shell ionization. In the adiabatic limit of low velocities, ξ is small compared to unity. The transferred momentum is then absorbed by the nucleus *via* the interaction with ejected electron, and since in a Coulomb potential, high moments are associated with small distances, the second factor in the matrix element effectively limits the spatial extension of the integration to the region $r_\perp \leqslant \frac{1}{q_0} = r_{ad}$.

This may be seen qualitatively from the expression for the Fourier component of the initial wave function of the K-shell electron, corresponding to z momentum $\hbar q_0$

$$\psi_0(r_\perp, q_z = q_0) \propto \int_{-\infty}^{\infty} dz \exp\left(-\sqrt{r_\perp^2 + z^2}/r_k + iq_0 z\right)$$

$$= r_k(1 + \xi^{-2}) \frac{r_\perp}{r_\xi} K_1\left(\frac{r_\perp}{r_\xi}\right) \qquad \ldots(5)$$

with

$$r_\xi = r_{ad}\, r_k/(r_{ad}^2 + r_k^2)^{1/2} = r_{ad}(1 + \xi^2)^{-1/2}$$

For small values of ξ, corresponding to $\bar{q}_0 > qK$ and $r_{ad} < r_k$ the dependence of the expression on $r_\perp$ is determine by r_{ad} only, $r_\xi \simeq r_{ad}$. The function K_1 is a modified Bessel function, and the product $\chi K_1(\chi)$ decreases monotonically from a value at unity at $x = 0$ with characteristic width ~ 1.

For ionization of a K-shell electron to the continuum, the final state $| n >$ may be any continuum state. At low velocities, however transitions to final states, with kinetic energy $T \ll E_B$ will be strongly favoured, and the quantitative arguments given above may be applied for a transition energy $\Delta E = E_B$ and the corresponding definition of r_{ad} and q_0.

As might be expected from equations (2) and (5), the impact parameter dependence of the ionization probability is governed by two lengths, r_{ad} and r_k. In fact, from more detailed calculation[9] a general approximate scaling law has been established,

$$I_p(P) = z_1^2/E_B\, f(\xi, \chi) \qquad \ldots(6)$$

with $\chi = P/r_{ad}$. In adiabatic limit, $\xi \to 0$ the function f approches the result obtained by Bang and Hansteen,[7] and the impact parameter dependence is determined by a unique function of χ. A convenient analytical expression has been given by Brant *et al.*[10] For finite values of ξ, the function may be obtained from published tables.[11] The simple scaling law (equation (6)) and the corresponding paramerization of theoretical results from the basis for treatment of correction to the first order Born approximation discussed below.

Corrections to First Order Born Approximation

At low projectile velocities, the agreement of experimental result with calculations based on the first order Born approximation is poor. This has been explained as being a result of several corrections, which become important in this limit. The three main effects, which will be discussed below, are corrections for binding, nuclear Coulomb repulsion, and relativistic effects.

Binding—At low velocities, the collision between projectile and target atom is nearly adiabatic, and a perturbation treatment should in principle be based on adiabatic perturbation theory, i.e., on a description with perturbed stationary states (pSS). The state of the bound electron is modified during the collision due to the proximity of the projectile nuclear charge. This modification was first introduced by Brant *et al.*[12] and they suggested that the main effect would be a change in electron binding energy which, for a projectile at distance R from the target nucleus and with charge Ze, may be evaluated to first order form,

$$\triangle E_B = \frac{Z_1 e^2}{R} [1 - (1 + R/r_k) \exp(-2R/r_k)]. \qquad ...(7)$$

The correction is seen to be important when the characteristic distance R are small compared to r_k, for $r_{ad}/r_k = \xi < 1$, which corresponds to the quasi-adiabatic region. The binding energy will according to equation[7] at the minimum distance of approach, $R_{\min}(P) \sim P$.

Coulomb Repulsion—At low velocities, the Coulomb repulsion from the target nucleus may modify significantly the projectile motion and thereby, the time dependence of the perturbation experienced by a K-shell electron. This effect was first treated by Bang and Hansteen[7] simple approximate correction to the total cross section for ionization,

$$\sigma_k \simeq \sigma_k^{s \cdot 1} \exp\left(-\frac{\pi}{2}\, b/r_{ad}\right), \qquad ...(8)$$

where b is the minimum distance of approach in a head-on collision, i.e.,

$$b = \frac{z_1 z_2 e^2}{E_{cm}}$$

in the corresponding energy E_{cm} in the centre of mass system. This estimate has been applied by Basbas *et al.*[13] with a small modification.

A systematic comparison with numerical calculation with hyperbolic projectile trajectories by Kobach[14] has revealed that eqn (8) is not very accurate, in particular when the parameter b/r_{ad} is not small, i.e., at very low velocities where the correction is large, also the correction only applies to total cross sections, and the dependence on impact parameter P, suggested by Bang and Hansteen[7] is rather complicated. Laegsgaard *et al.*[15] attempted to drive a simple prescription for the repulsion correction determined by

$$E_{cm} \rightarrow E_{cm} - z_1 z_2 e^2/R, \qquad ...(9)$$

where the distance R is given by,

$$R = (R_{\min}(P)^2 + r_{ad}^2)^{1/2} \qquad ...(10)$$

Relativistic effect—A relativistic (SCA) treatment of K-ionization is given by Amundsen *et al.*[16] The monopole contribution to the ionization probability $I(P)$ may be obtained by integration over final electron energy E_f.

At low velocities ($\xi \ll 1$), the monopole contribution dominates, and such a calculation should yield a good approximation to the total ionization probability.

Results and Discussion

In general, it is diffcult from a comparison with experiment to draw any conclusions about the treatment of the individual correction since errors in these may cancel. However, to some extent we avoid this problem by comparing the calculated and measured ratio of cross sections as shown in Fig. 1 for K-shell ionization of Ag by protons, deuterons, and α-particles, experimental data taken from Hogedal.[17] For fixed projectile velociiy and charge-to mass ratio Z_1/M_1, the correction to the

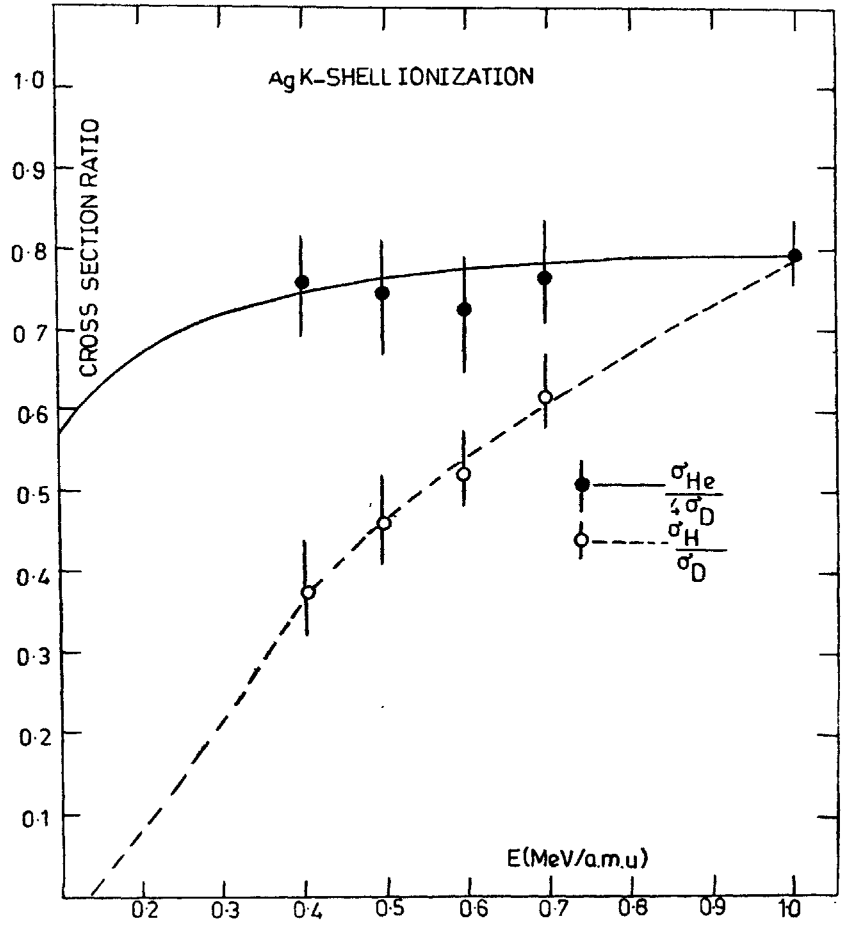

FIG 1 Ratio of Silver *K*-shell ionization crosssections for helium-deuteron and hydrogen-deuteron ions.

● experimental data ratio for $\sigma_\alpha/4\sigma_\alpha$ add————theoretical one,

○ experimental data ratio for σ_p/σ_d and- - - - - - - - - -theoretical one, theoretical curves calculated using (SCA-B-C-R).

ionization cross section for nuclear Coulomb repulsion should be nearly the same, while the correction for binding will vary with the charge Z_1 and lead to a diviation from scaling with Z_1^2. The comparison in Fig. 1 with ratios of ionization cross sections for α-particles and deuterons is therefore, a test of mainly the binding correction, although the three major corrections were included in the calculations (B; C and R). Similarly, the ratio of cross sections for nuclear Coulomb repulsion is a function of charge-to-mass ratio for both cases, the agreement with experiment is satisfactory. It may be noted that a correction for Coulomb repulsion based on equation (8) is in poor agreement with the data, from being much to very small at the lower velocities.

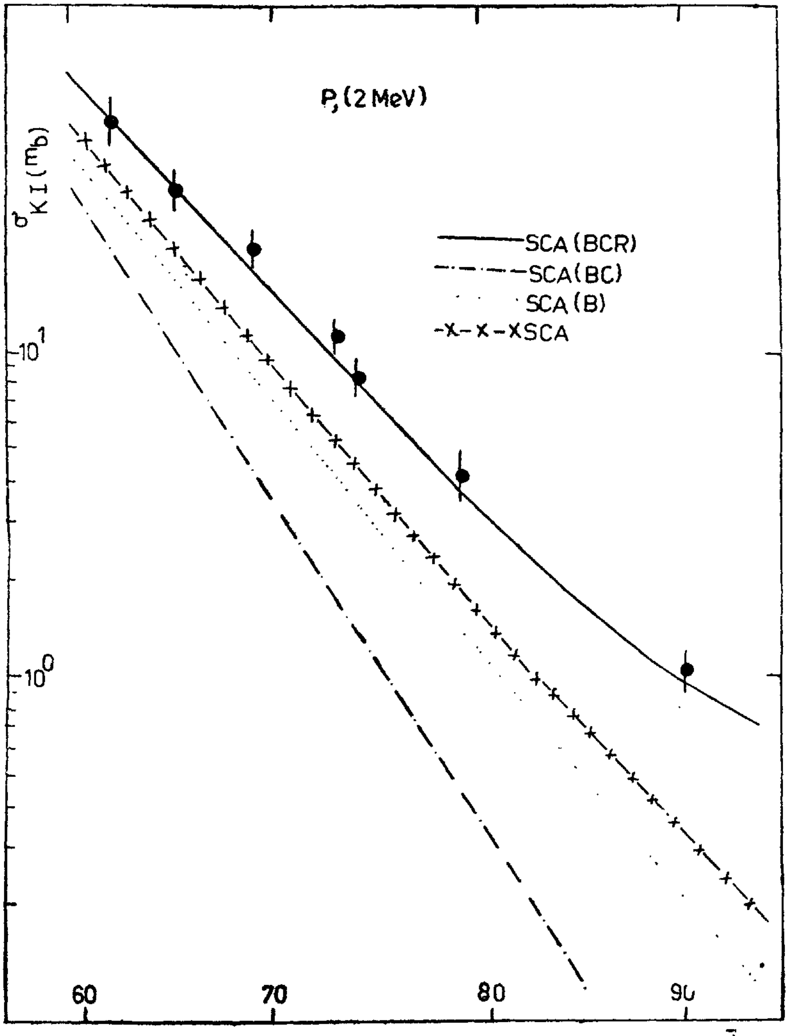

FIG 2 Dependence on target nuclear charge Z_2 of 2MeV protons induced K-shell ionization. The curves correspond to results at the various stages in the correction procedure.

The relativistic correction is important mainly for high target atomic number Z_2 and may be tested by a comparison with experiment of the calculated dependence of the crossection on Z_2 for fixed projectile energy, $E_P = 2$MeV, as shown in Fig. 2 *vide* the experimental points taken.[2-5,18,19] The theoretical curves give the (SCA) predictions uncorrected (SCA), including the binding correction (SCA-B), including both binding and Coulomb crrection (SCA-B-C) and finally including also the relativistic correction (SCA-B-C-R). For high Z_2, the latter correction dominates. The good agreement with measured crosssections suggests that the simple correction procedure may useful in connection with application of proton-induced X-ray emission (PIXE) analysis.

The relativistic correction also depends strongly on the projectile velocity, becoming very large in the limit of low velocities. A comparison with experiment, testing this dependence, is shown in Fig. 3 based on experimental data[19-22] the dominant corrections are those for the relativistic effects and for Coulomb repulsion the latter introducing an effective threshold for ionization. The calculation overestimate the crosssection at higher energies, but the overall agreement is satisfactory. It may be noted that at the lowest energies, the measured X-ray yields were corrected for contributions from nuclear Coulomb excitation ($\leqslant$ 7 per cent).

From a comparison with experiment, the simple correction procedure appears to be quite accurate even when the corrections are very large. Since the prescrip-

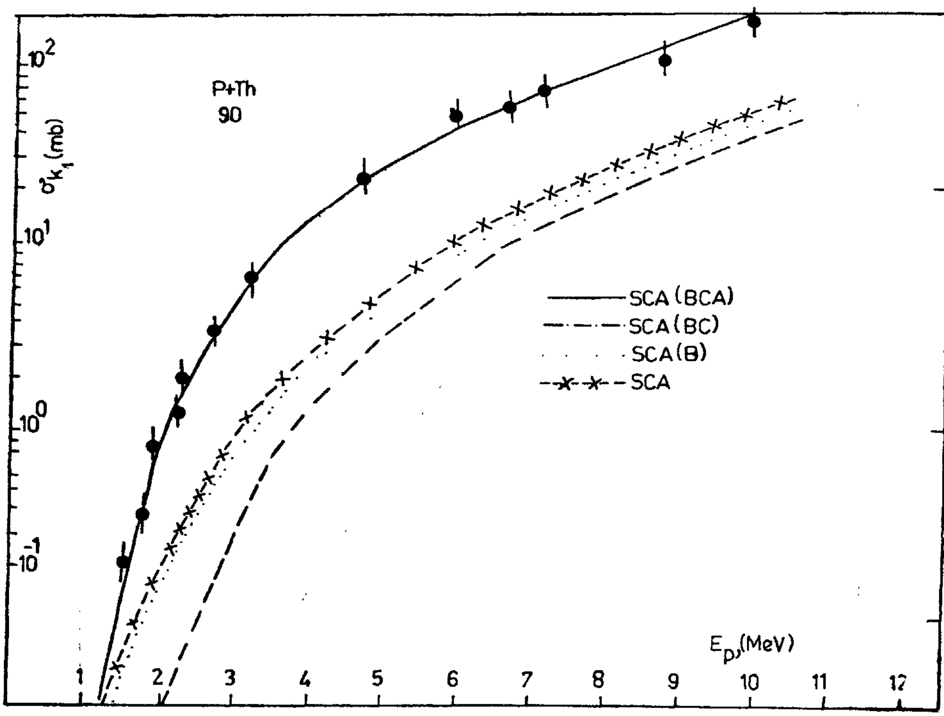

FIG 3 Proton-induced *K*-shell ionization in Th in this energy range ($\xi < 0.5$).

tions are based on scaling properties of the ionization probability rather than on some kind of perturbation expansion, the corrections are still meaningful for such cases, but their accuracy is somewhat uncertain. An extreme example is shown in Fig. 4, experimental data taken from Zelasny and Hornshoj.[24] All the corrections are very large, but the final result agrees with experiment. It may be noted that for such a case the order of the sequences of corrections is very important. Thus the relativistic corrections are much larger for the united atom $_{80}$Pb, than they are for $_{74}$W. The close agreement may to some extent be fortuitous but still indicates that the basic phenomenon responsible for the observed X-ray production is simple ionization. While the corrections for Coulomb repulsion and for relativistic

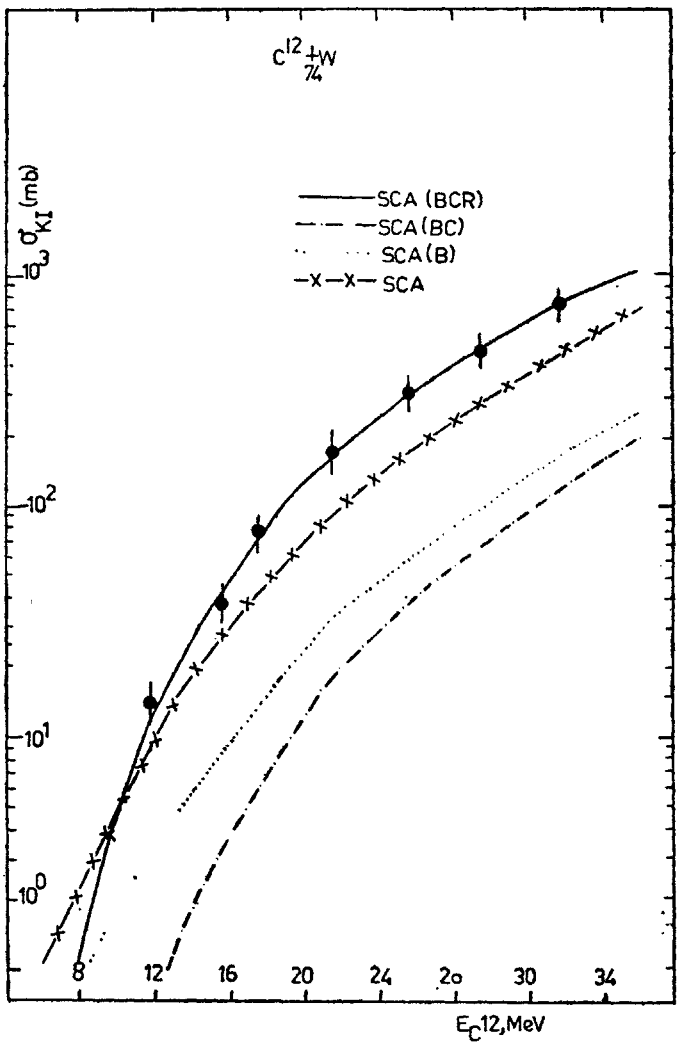

FIG 4 Tangeston *K*-shell ionization crosssection for incident Carbon ions

effect should be applicable for high projectile velocities, the treatment of binding applies only to the region of low projectile velocities; $\xi \leqslant 1$.

In conclusion, the present data show the need for binding, Coulomb, and relativistic corrections in the calculation of cross-section for heavy elements. Their inclusion in the (SCA) gives the most satisfactory agreement with experiments.

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