Polarization and binding effects in K-shell ionization by ^{16}O and ^{32}S ions

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The theoretical model of Montenegro and Sigaud is used for the description of the experimental total K-shell ionization cross sections for 2.2-MeV/u ^{16}O and ^{32}S on 24 targets from $_{21}Sc$ to $_{83}Bi$ obtained by Seidel *et al.* The predictions of the model, which considers both binding and static polarization effects within the framework of adiabatic perturbation theory, are very good for the majority of the measured data in the region of validity of the model. The electron-capture process that can contribute in the region of the largest values of relative velocity ξ_K is also analyzed.

In a recent paper, Seidel *et al.*[1] presented total and impact-parameter-dependent K-shell ionization cross-section measurements with ^{16}O and ^{32}S ions of 2.2 MeV/u on a wide range of targets. These data span the transition region from very asymmetric slow ($\xi_K \ll 1$) collisions to almost symmetric and fast ($\xi_K \simeq 1$) collisions, so the changing role of the transient binding and polarization of the wave function of the active electron can be studied. Here, as in Ref. 1, we characterize the collisions by the usual[2] relative impact-velocity parameter ξ_K. It was found in Ref. 1 that it is ξ_K alone which controls the transition from the united-atom (UA) binding situation for $\xi_K \ll 1$ to the separated-atom (SA) binding situation for fast collisions, $\xi_K \simeq 1$. The approximate static two-center model of transient binding by Andersen *et al.*[3] very successfully describes[1] a large set of data for $\xi_K < 0.6$. It fails, however, to reproduce the pronounced rise of the K-shell cross sections above the relativistic semiclassical approximation (RSCA), (Ref. 4) with UA binding in the nonadiabatic regime near $\xi_K \simeq 1$. Here, the contributions from large impact parameters to the K-shell cross section become dominant and, therefore, polarization effects are expected to be large. We shall, in this paper, focus attention on these nonadiabatic collisions.

In a previous paper, Montenegro and Sigaud[5] used the adiabatic perturbation theory to study the ionization of the $1s\sigma$ molecular orbital. They extended this model to nonadiabatic systems like those studied in Ref. 1 by imposing an asymptotic matching with the semiclassical approximation through an effective charge which, besides simulating the relaxation of the active and passive electrons, connects this relaxation to the evolution of the center of charge during the collision process. These authors treated[6] the polarization effects for collisions with $\xi_K < 1$, where the projectile velocity remains below about one-half the K-shell Bohr velocity, in a static approximation which takes account of the separation between the center of charge and the target. This approximation appears justified, and a substantial improvement is expected in reproducing the cross-section data of Ref. 1 for $\xi_K > 0.6$. This is the velocity range where the model of Andersen *et al.*[3] fails. For relative velocities $\xi_K < 0.6$ we expect only minor changes when using the present model.[5,6]

We compare in Fig. 1 both the model of Montenegro

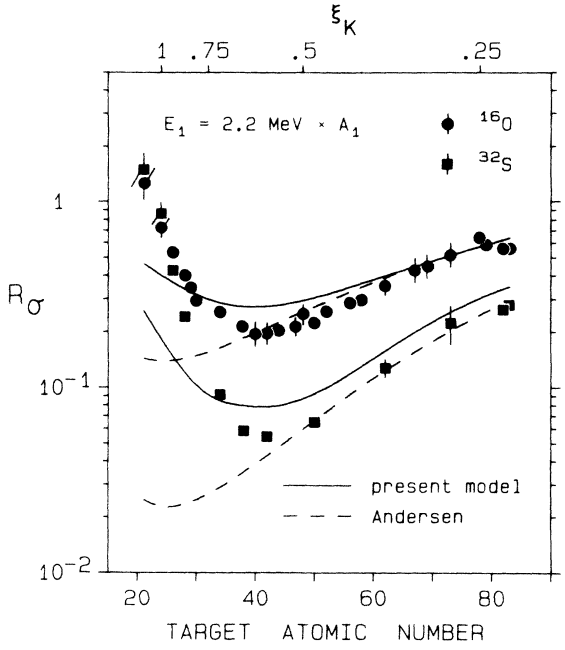

FIG. 1. Ratios R_σ of reduced cross sections, as defined in the text, for ^{16}O and ^{32}S projectiles of 2.2 MeV/u. Theoretical ratios are calculated using the model of Montenegro and Sigaud (Refs. 5 and 6) (solid curves) and Andersen *et al.* (Ref. 3) (dashed curves).

and Sigaud[5,6] and the calculations following Andersen *et al.*[3] to the ^{16}O and ^{32}S induced K-shell ionization cross sections σ_K. We plot them in the form of reduced ratios for projectile charge Z_1,

$$R_\sigma(Z_1)=\sigma_K(Z_1)/Z_1^2\sigma_K^{\mathrm{RSCA}}(^2_1\mathrm{H}) ,$$

where $\sigma_K(^2_1\mathrm{H})$ serves as reference cross section.[1] While the theoretical curves remain almost unchanged for $\xi_K<0.5$, a substantial improvement is observed for $0.5<\xi_K<1.2$ which we attribute to an adequate treatment of polarization effects. The improvement over the frequently employed united-atom binding approximation is even more dramatic: for instance, the discrepancy between experimental and theoretical K-shell cross sections[1] of $_{21}$Sc ($\xi_K\simeq 1.2$) is reduced from a factor of 17 to a factor of 2.8 for ^{16}O projectiles, and from a factor of 180 to a factor of 5.8 for ^{32}S. Yet, as this example and Fig. 1 show, the theory[5,6] still does not reproduce the data quantitatively in the region of the minimum of R_σ, and for the highest ξ_K. We note, however, that over the ξ_K range of Fig. 1, the σ_K themselves change by 6 orders of magnitude[1] for ^{16}O as well as ^{32}S projectiles, so that the R_σ plotted in this figure strongly emphasize the remaining discrepancies. These tend to increase systematically for more symmetric collisions, as revealed by the comparison of ^{16}O and ^{32}S data at equal relative velocity ξ_K.

The reasons for the remaining differences may be sought in two directions:

(i) The ^{32}S data for targets lighter than $_{28}$Ni reach into the $Z_1/Z_2>0.5$ region where we do not expect the model of Refs. 5 and 6, which is based on direct Coulomb ionization from the $1s\sigma$ molecular orbital, to be valid.[7]

(ii) The cross sections for ^{16}O on Cr and Sc targets were measured in Ref. 1 with both very thin and medium-thickness targets, and with different charge states of the ^{16}O projectiles. The comparison revealed a 50% decrease in the measured cross section when the projectile charge state was lowered from 7^+ to 5^+ and thin targets were used. In the 5^+ charge state, the K electrons are kept with the projectile, and the K-K capture channel, which is the most important one for the creation of K-shell vacancies in the target, is inhibited. The cross sections are then close to those for Coulomb ionization. When thicker targets are used, the projectile charge state reaches the equilibrium value of 7^+ for 35-MeV ^{16}O ions,[8] thus opening the K-K capture channel. We assume for simplicity that for those collisions the K-K capture channel is completely open and is the only one to contribute. With this assumption, an estimate of the capture cross section can be made by using the OBK-Nikolaev approximation in the version presented by Lapicki and McDaniel.[9] The result of this calculation, when added to the direct Coulomb ionization,[5,6] gives rise to the dashed curve in Fig. 2. Good agreement with the data is thus obtained.

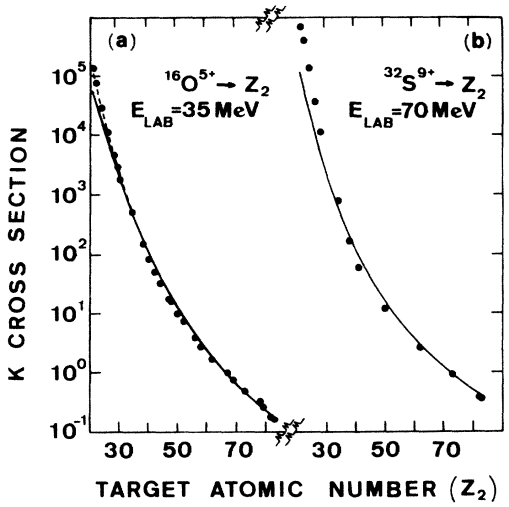

FIG. 2. (a) Comparison between the experimental total K-shell ionization cross sections (in barns) for 2.2-MeV/u $^{16}O^{5+}$ ions obtained by Seidel *et al.* (Ref. 1) and the theoretical model of Montenegro and Sigaud (Refs. 5 and 6) (solid line). The dashed curve represents the sum of the results obtained in this model and K-K electron capture calculations based on the OBK-Nikolaev approximation (see text). (b) Same as in (a) but for 2.2-MeV/u $^{32}S^{9+}$ ions. No K-K electron capture is added.

A similar attempt to add in the K-K electron-capture cross section does not appear very meaningful for the ^{32}S data. Firstly, the calculation of Coulomb ionization according to the model of Montenegro and Sigaud[5,6] is quantitatively unreliable for the targets below $_{28}$Ni, as stated above. Secondly, with an average charge state[8] of 12^+ of 70-MeV ^{32}S ions in the target, the K-K capture channel is strongly inhibited, in contrast to the situation with the ^{16}O data. We believe that both the insufficient knowledge of the charge-state distribution of ^{32}S in the target and the very approximate nature of the OBK-Nikolaev estimate[9] preclude at present a further elucidation of the remaining discrepancy.

The foregoing discussion has shown that the model of Coulomb ionization of the $1s\sigma$ orbital, extended[5,6] to asymmetric and nonadiabatic collisions, successfully describes the onset of polarization effects on K-shell ionization cross sections in heavy-ion collisions. The complex situation near the borderline of validity of the model, however, demands quantitative clarification.

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[1] J. Seidel, S. Röhl, R. Lorek, S. Huchler, and M. Dost, Phys. Rev. A 32, 2142 (1985).

[2] G. Basbas, W. Brandt, and R. Laubert, Phys. Rev. A 7, 983 (1973).

[3] J. U. Andersen, E. Laegsgaard, and M. Lund, Nucl. Instrum. Meth. 192, 79 (1982).

[4] F. Rösel, D. Trautmann, and G. Baur, Nucl. Instrum. Meth. 192, 43 (1982) and references therein.

[5]E. C. Montenegro and G. M. Sigaud, J. Phys. B **18**, 299 (1985).
[6]E. C. Montenegro, A. G. de Pinho, and G. M. Sigaud, J. Phys. B (to be published).
[7]D. Madison and E. Merzbacher, in *Atomic Inner-Shell Processes,* edited by B. Crasemann (Academic, New York, 1975), Vol. I, p. 1.
[8]A. B. Wittkower and H. D. Betz, At. Data **5**, 113 (1973); E. C. Montenegro, S. A. Cruz, and C. Vargas-Aburto, Phys. Lett. **92A**, 195 (1982).
[9]G. Lapicki and F. D. McDaniel, Phys. Rev. A **22**, 1986 (1980).