Technical Physics Letters, Vol. 29, No. 9, 2003, pp. 760–763. Translated from Pis'ma v Zhurnal Tekhnicheskoĭ Fiziki, Vol. 29, No. 18, 2003, pp. 29–36.

K-Shell Ionization of a Quasirelativistic Hydrogenlike Atom upon Collision with a Relativistic Structural Multiply Charged Ion

V. I. Matveev*, E. S. Gusarevich, and I. N. Pashev
Pomorskiĭ State University, Arkhangelsk, Russia
Arkhangelsk State Technical University, Arkhangelsk, Russia
** e-mail: matveev.victor@pomorsu.ru*
Received March 11, 2003

Abstract—The differential and total ionization cross sections of a heavy hydrogenlike atom colliding with a relativistic structural heavy ion are calculated using a relativistic generalization of the method of solution matching and the eikonal approximation. By structural ions are implied partly stripped ions of heavy elements comprising a nucleus and a certain number of bound electrons partly compensating for the nuclear charge. The heavy target atom is described using quasirelativistic wave functions. It is shown that an allowance for relativistic effects in the heavy target atom leads to significant changes in the ionization cross sections as compared to those determined within the framework of a nonrelativistic description. *© 2003 MAIK "Nauka/Interperiodica".*

Experimental investigations of collision processes involving heavy ions possessing high charges and energies frequently involve partly stripped ions (see, e.g., [1–7] and references therein). In the calculations schemes used to describe the process of excitation and ionization of target atoms, such ions are usually considered as point charges. A relatively small number of investigations were devoted to development of the calculation schemes describing partly stripped ions as finite-size charged particles with a certain electron structure. The strong field of the multiply charged ion hinders using the perturbation theory. For this reason, the ionization cross sections have usually been performed (see, e.g., [8, 9]) within the framework of the well-known method of classical trajectories. The quantum-mechanical description based on a sudden perturbation approximation attempted by Yudin [10, 11] only allowed the ionization probabilities to be determined within a limited interval of impact parameters.

Previously [12, 13], the energy losses in the collisions of relativistic structural heavy ions with light (nonrelativistic) atoms were calculated using the eikonal approximation. Recently [14], we used the same approach to calculate the cross sections of the single and double ionization of hydrogenlike and heliumlike atoms. The results obtained in [14] can be used for calculating the cross sections of the formation of single and double vacancies in the *K*-shells of only light atoms. In calculating the cross section of analogous inelastic processes in heavy atoms, it is necessary to take into account the relativistic character of the motion of electrons both in the bound states and in the continuum.

In this study, we have developed a nonperturbative method for calculating the ionization cross sections of heavy quasirelativistic hydrogenlike target atoms interacting with partly stripped relativistic multiply charged ions considered as extended charges. The proposed method is based on a relativistic generalization [15, 16] of the method of solution matching and the eikonal approximation and on their extension to the case of extended charges proposed previously [12, 17]. For illustration, the proposed method is applied to calculation of the total and differential ionization cross sections. It will be shown that an allowance for the relativistic effects leads to significant changes in the total and differential ionization cross sections as compared to those determined within the framework of a nonrelativistic description of the target. These changes are substantial only in the case of targets with large nuclear charges. It should be noted that we decline from discussing the processes of excitation and loss of electrons belonging to the projectile ions, which are now under extensive experimental and theoretical investigation (see, e.g., [2, 18]).

Consider a hydrogenlike atom at rest at the origin of coordinates. According to [15, 16], the differential cross section for the ionization of this atom, whereby it passes from the ground state $|0\rangle$ (with the energy E_0) into state $|\mathbf{k}\rangle$ in the continuum (with the momentum $\mathbf{k}$ and energy $E_{\mathbf{k}}$) upon collision with a relativistic ion possessing the nuclear charge Z and moving at the velocity $\mathbf{v}$ can be described in the eikonal approximation as (here and below, we use the atomic system of units where $\hbar = e = m_e = 1$, $\hbar$ being the Planck constant, e the electron charge, and m_e the electron mass)

1063-7850/03/2909-0760$24.00 © 2003 MAIK "Nauka/Interperiodica"

$$d\sigma = \int d^2\mathbf{b}\left|\left\langle \mathbf{k}\left|\left[1-\exp\left(-\frac{i}{v}\int U dX\right)\right]\gamma^{-1}S^2\exp\left\{i\frac{xv}{c^2}(E_\mathbf{k}-E_0)\right\}\right|0\right\rangle\right|^2 d^3\mathbf{k}. \quad (1)$$

In this relation, $\mathbf{b}$ is the impact parameter, $S^2 = \gamma(1 - \boldsymbol{\alpha\beta})$, $\gamma = (1 - \boldsymbol{\beta}^2)^{-1/2}$, $\boldsymbol{\beta} = \mathbf{v}/c$, $\boldsymbol{\alpha}$ are the Dirac matrices. and c is the velocity of light in vacuum (the x axis is directed along the ion velocity).

The scattering Coulomb potential $U = U(X, \mathbf{b}; \mathbf{r})$ is considered as a function of both the ion coordinates $\mathbf{R} = (X, \mathbf{b})$ and the positions of the atomic electron $\mathbf{r} = (x, \mathbf{s})$, where $\mathbf{s}$ is the projection of $\mathbf{r}$ onto the plane of the impact parameter $\mathbf{b}$. According to [12, 14], the eikonal phase in formula (1) can be represented as

$$-\frac{i}{v}\int U dX = i\mathbf{qs},$$

where

$$\mathbf{q} = \frac{2Z^*}{vb}\left[1+\frac{\nu}{1-\nu}\frac{b}{\lambda}K_1\left(\frac{b}{\lambda}\right)\right]\frac{\mathbf{b}}{b}.$$

Here, the vector $\mathbf{q}$ has an evident meaning of the momentum transfer to the atomic electron from a structural projectile ion with an impact parameter $\mathbf{b}$, $K_1(x)$ is the Macdonald function, $Z^* = Z(1 - \nu)$ is the effective (apparent) ion charge, $\nu = N_i/Z$ is the relative number of electrons in the ion coat, N_i is the total number of electrons in the shells, λ is the screening parameter (or the effective ion radius). The latter quantity is given by the formula $\lambda = g\nu^{2/3}(1 - \nu/7)^{-1}Z^{-1/3}$ where $g \approx 0.48$ [19].

Formula (1) for the ionization cross section was derived [15, 16] based on a relativistic generalization of the eikonal approximation taking into account the relativistic character of motion for both the impinging ion and the target atom. However, the calculations performed previously (see, e.g., [14]) for the cross sections of ionization by impact of a structural heavy ion took into account only the relativistic motion of the projectile ion.

In this study, we allow for the relativistic effects in the target atom as well. For this calculation, the wave functions in the initial ($|0\rangle$) and final ($|\mathbf{k}\rangle$) states will represent (as in [20, 21]) the quasirelativistic wave functions determined according to Darwin [22–24]:

$$|0\rangle \equiv \Psi_{0,s}(\mathbf{r}) = N_0\left(1-\frac{i}{2c}\boldsymbol{\alpha}\nabla\right)\phi_0(\mathbf{r})u_s,$$

$$|\mathbf{k}\rangle \equiv \Psi_{\mathbf{k},s'}(\mathbf{r}) = N_1\left(1-\frac{i}{2c}\boldsymbol{\alpha}\nabla\right)\phi_\mathbf{k}(\mathbf{r})u_{s'},$$

$$\phi_\mathbf{k}(\mathbf{r}) = (2\pi)^{-3/2}\exp\left(\frac{\pi\xi}{2}\right)\Gamma(1+i\xi) \quad (2)$$

$$\times\exp(i\mathbf{kr})F(-i\xi, 1, -i(kr+\mathbf{kr})),$$

$$\phi_0(\mathbf{r}) = \sqrt{Z_a^3/\pi}\exp(-Z_a r).$$

Here, ϕ_0 and $\phi_\mathbf{k}$ are the nonrelativistic wave functions of the ground state and continuum for a hydrogenlike atom with a nuclear charge Z_a, $\xi = Z_a/k$, $\Gamma(x)$ is the gamma function, $F(\alpha, \gamma, z)$ is the degenerate hypergeometric function, u_s is the bispinor of a resting electron with the spin projection s, and $N_1 = (1 + (k/2c)^2)^{-1/2}$ and $N_0 = (1 + (Z_a/2c)^2)^{-1/2}$ are the normalization factors (see, e.g., [20, 21]). Following [16, 17], we assume for the quasirelativistic atom that $\exp\{ixv(E_k - E_0)/c^2\} \approx 1$ and $\gamma^{-1}S^2 \approx 1$.

Using the method of solution matching [14–16], we obtain an expression for the differential cross section of electron emission with the energy ε_k in the following form:

$$\frac{d\sigma}{d\varepsilon_k} = 8\pi\frac{Z^{*2}}{\mathbf{v}^2}\lambda_k k\left(\ln\frac{2Z_a\alpha_k\mathbf{v}^2\gamma}{\eta Z^*\omega_k}-\frac{\beta^2}{2}\right). \quad (3)$$

Here, $\eta = \exp B = 1.781$, $B = 0.5772$ is the Euler constant, $\omega_k = \varepsilon_k - \varepsilon_0$, $\varepsilon_k = k^2/2$, and $\varepsilon_0 = -Z_a^2/2$. The quantities λ_k and α_k are given by the formulas (cf. [14, 15])

$$\lambda_k = \frac{1}{3}(N_1N_0)^2\int|\langle\phi_\mathbf{k}|\mathbf{r}|\phi_0\rangle|^2 d\Omega_\mathbf{k},$$

$$\alpha_k = \lim_{b_0\to\infty}\frac{Z^*}{\mathbf{v}Z_a b_0}$$

$$\times\exp\left\{\frac{1}{\lambda_k}\frac{\mathbf{v}^2}{8\pi Z^{*2}}(N_1N_0)^2\int_0^{b_0}2\pi b\,db\int d\Omega_\mathbf{k}|\langle\phi_\mathbf{k}|\exp(i\mathbf{qr})|\phi_0\rangle|^2\right\},$$

where $\Omega_\mathbf{k}$ is the solid angle of the momentum vector $\mathbf{k}$ of the emitted electron. In the formulas for λ_k and α_k, the integration is performed over all $\Omega_\mathbf{k}$.

We have used formula (3) to calculate the differential cross section (spectrum) of electron emission from a hydrogenlike atom of molybdenum Mo^{41+} colliding with a relativistic uranium ion U^{50+}. The results of this calculation are presented in Fig. 1. For evaluating the contribution of relativistic effects to the differential ionization cross section of a heavy hydrogenlike atom, it is convenient to introduce a relative correction $\chi = [(d\sigma/d\varepsilon_k)_n - (d\sigma/d\varepsilon_k)_r]/(d\sigma/d\varepsilon_k)_n = 1 - (N_0N_1)^2$, where indices n and r indicate the nonrelativistic and relativistic descriptions, respectively. Thus, the correction χ in the quasirelativistic approach is given by a simple formula depending only on the nuclear charge Z_a of the target and on the emitted electron energy ε_k. At the same time, the correction is independent of the energy

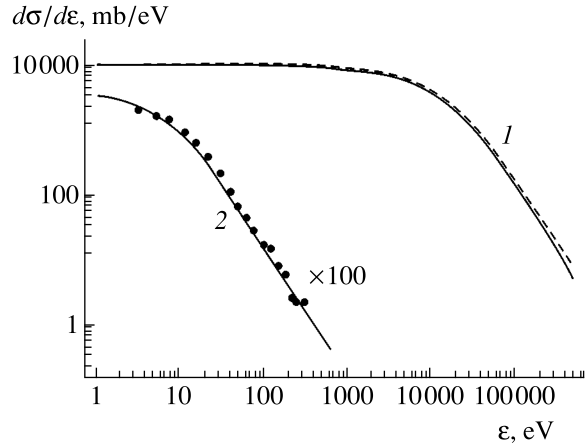

Fig. 1. Plots of the ionization cross section versus the emitted electron energy ε: (*1*) for a structural U^{50+} ion (projectile) with an energy of 10000 MeV/nucleon colliding with a hydrogenlike Mo^{41+} target atom (solid and dashed curves correspond to a quasirelativistic and nonrelativistic descriptions of the target, respectively); (*2*) for a stripped C^{6+} ion with an energy of 2.5 MeV/nucleon colliding with a hydrogen atom (solid curve shows the results of calculations, black circles represent the experimental data [25]; both calculated and experimental values are multiplied by a factor of 100).

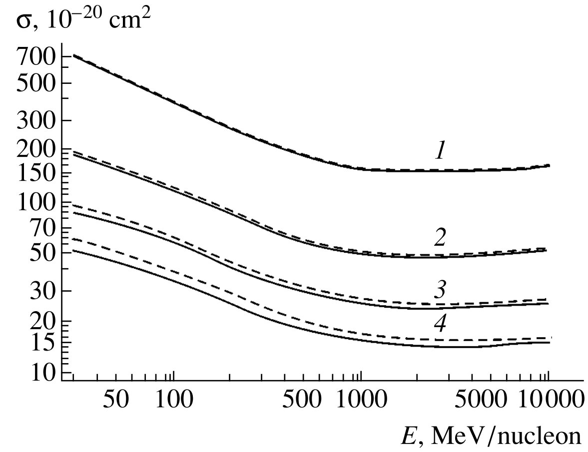

Fig. 2. Plots of the total ionization cross section for various hydrogenlike target atoms versus the energy of the impinging U^{50+} ion (solid and dashed curves correspond to a quasirelativistic and nonrelativistic descriptions of the target, respectively): (*1*) Mg^{11+} (Z_a = 12); (*2*) Ti^{21+} (Z_a = 22); (*3*) Ge^{31+} (Z_a = 32); (*4*) Mo^{41+} (Z_a = 42).

and charge of the impinging ion. As the emitted electron energy grows, the correction increases. For example, in a Mo^{41+} target, χ = 2.31% and 11.1% for the electron energies ε_k = 100 eV and 100 keV, respectively. Unfortunately, no experimental data are available on the electron spectra for the *K*-shell ionization of heavy hydrogenlike atoms by structural heavy relativistic ions in the range of energies and charges under consideration. For this reason, we illustrate the results obtained using the proposed method in the case of insignificant relativistic effects in the target. For this purpose, Fig. 1 shows the electron emission spectrum calculated using formula (3) for a hydrogen atom colliding with stripped carbon ions in comparison to the experimental data reported in [25].

The total ionization cross section of a hydrogenlike heavy target is obtained by integrating expression (3) over the entire interval of energies of the emitted electron. According to the method of solution matching [14, 15], this is equivalent to calculation of the following values:

$$\lambda_i = \int_0^\infty \lambda_k k^2 dk, \quad \omega_i = \exp\left\{\frac{1}{\lambda_i}\int_0^\infty k^2\lambda_k \ln\omega_k dk\right\},$$
$$\alpha_i = \exp\left\{\frac{1}{\lambda_i}\int_0^\infty k^2\lambda_k \ln\alpha_k dk\right\}. \tag{4}$$

In these terms, the total ionization cross section is expressed as

$$\sigma = 8\pi\frac{Z^{*2}}{\mathbf{v}^2}\lambda_i\left(\ln\frac{2Z_a\alpha_i\mathbf{v}^2\gamma}{\eta Z^*\omega_i} - \frac{\beta^2}{2}\right). \tag{5}$$

Figure 2 gives an example of using formula (5) for calculating the total ionization cross section of a hydrogenlike target atom as a function of the energy of impinging U^{50+} ions for several values of the nuclear charge of the target. As can be seen from these data, allowance for relativistic effects in the target leads to a decrease in the total ionization cross section as com-

The relative contribution η of the relativistic effects determined as a function of the energy *E* [MeV/nucleon] of a relativistic structural ion U^{50+} colliding with hydrogenlike atoms of Mg^{11+} (Z_a = 12), Ti^{21+} (Z_a = 22), Ge^{31+} (Z_a = 32) and Mo^{41+} (Z_a = 42)

E, MeV/n	50	100	500	1000	5000	10000	50000	100000
η, % (Z_a = 12)	1.5	1.4	1.1	1.0	0.9	0.9	0.8	0.7
η, % (Z_a = 22)	4.6	3.9	3.0	2.8	2.5	2.4	2.2	2.1
η, % (Z_a = 32)	8.2	6.9	5.4	5.0	4.6	4.4	4.1	4.0
η, % (Z_a = 42)	12.0	10.1	8.1	7.6	7.0	6.8	6.4	6.2

pared to that obtained in the nonrelativistic description. The relative contributions of the relativistic effects determined as $\eta = [\sigma_n - \sigma_r]/\sigma_n$ are given in the table, where indices n and r refer to the nonrelativistic and relativistic descriptions of the target, respectively. In accordance with formulas (4) and (5), the values of η depend on the characteristics of both the target and the projectile.

Acknowledgments. This study was supported by the Russian Foundation for Basic Research (project no. 01-02-17047) and by the Ministry of Education of the Russian Federation (project no. E02-3.2-512).

REFERENCES

1. H. F. Krause, C. R. Vane, S. Datz, *et al.*, Phys. Rev. A **63**, 032711 (2001).
2. T. Ludziejewski, Th. Stohlker, D. C. Ionescu, *et al.*, Phys. Rev. A **61**, 052706 (2000).
3. E. Wells, I. Ben-Itzhak, K. D. Carnes, *et al.*, Phys. Rev. A **60**, 3734 (1999).
4. M. Tschersich, R. Drozdowski, M. Busch, *et al.*, J. Phys. B **32**, 5556 (1999).
5. M. B. Shah and H. B. Gilbody, J. Phys. B **16**, L449 (1983).
6. J. H. McGuire, A. Mueller, B. Schuch, *et al.*, Phys. Rev. A **35**, 2479 (1987).
7. H. Berg, J. Ullrich, E. Bernstein, *et al.*, J. Phys. B **25**, 3655 (1992).
8. M. Purkait, A. Dhara, S. Sounda, *et al.*, J. Phys. B **34**, 755 (2001).
9. C. Illescas, B. Pons, and A. Riera, Phys. Rev. A **63**, 062722 (2001).
10. G. L. Yudin, Dokl. Akad. Nauk SSSR **282**, 874 (1985) [Sov. Phys. Dokl. **30**, 488 (1985)].
11. G. L. Yudin, Zh. Tekh. Fiz. **55**, 9 (1985) [Sov. Phys. Tech. Phys. **30**, 4 (1985)].
12. V. I. Matveev, Zh. Éksp. Teor. Fiz. **121**, 260 (2002) [JETP **94**, 217 (2002)].
13. V. I. Matveev, Zh. Tekh. Fiz. **72** (5), 10 (2002) [Tech. Phys. **47**, 523 (2002)].
14. V. I. Matveev and E. S. Gusarevich, Zh. Éksp. Teor. Fiz. **123**, 42 (2003) [JETP **96**, 34 (2003)].
15. V. I. Matveev and Kh. Yu. Rakhimov, Zh. Éksp. Teor. Fiz. **114**, 1646 (1998) [JETP **87**, 891 (1998)].
16. V. I. Matveev, D. U. Matrasulov, and Kh. Y. Rakhimov, J. Phys. B **32**, 3849 (1999).
17. V. I. Matveev and D. U. Matrasulov, J. Phys. B **33**, 2721 (2000).
18. A. B. Voitkiv, C. Muller, and N. Grun, Phys. Rev. A **66**, 062701 (2000).
19. W. Brandt and M. Kitagawa, Phys. Rev. B **25**, 5631 (1982).
20. R. Anholt, Phys. Rev. A **19**, 1004 (1979).
21. D. M. Davidovic, B. L. Moiseivitsch, and P. H. Norrington, J. Phys. B **11**, 847 (1978).
22. C. G. Darwin, Proc. R. Soc. London, Ser. A **118**, 654 (1928).
23. J. Eichler and W. E. Meyrhoft, *Relativistic Atomic Collisions* (Academic, New York, 1995).
24. V. B. Berestetskii, E. M. Lifshitz, and L. P. Pitaevskii, *Course of Theoretical Physics*, Vol. 4: *Quantum Electrodynamics* (Nauka, Moscow, 1989; Pergamon, New York, 1982).
25. L. C. Tribedi, P. Richard, L. Gulyás, *et al.*, Phys. Scr. **T80**, 333 (1999).

Translated by P. Pozdeev