L-SHELL IONIZATION PROBABILITIES IN NEAR CENTRAL HEAVY ION-ATOM COLLISIONS*

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The average L-shell ionization probabilities in near central collisions were determined from the Kα X-ray satellite yield distributions measured for elements with $42 \leq Z_{\rm target} \leq 92$ bombarded by N, O, and Ne ions. A comparison of experimental values with Semiclassical Approximation (SCA-HYD) and Classical Trajectory Monte Carlo (CTMC) calculations shows the importance of the electron capture mechanism for reduced velocities $\eta \simeq 1$. The CTMC calculations of direct ionization plus electron capture are in agreement with experimental L-shell ionization probabilities.

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There are two main mechanisms which contribute to the inner shell ionization in the intermediate energy heavy ion–atom collisions: the direct

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Coulomb ionization (DI) and the electron capture (EC) to the vacant shells of the projectile. Because of the many body nature of these processes, the full quantum mechanical description is rather difficult and requires large scale numerical computations. For this reason several semiclassical or classical models have been developed. In this paper we present our preliminary results concerning the applicability of Semiclassical Approximation (SCA--HYD) and Classical Trajectory Monte Carlo (CTMC) theories for the description of heavy ion induced ionization of medium heavy and heavy target atoms. The SCA-HYD and CTMC calculations are compared with experimental L-shell ionization probabilities for near central collisions of ^{14}N, ^{16}O, and ^{20}Ne ions with $_{42}$Mo, $_{46}$Pd, $_{57}$La, $_{60}$Nd, $_{65}$Tb, $_{73}$Ta, $_{92}$U targets. The experimental data were obtained from measurements carried out with the use of bent crystal spectrometer facilities at KVI-Groningen, KFA-Jülich and PSI-Villigen [1–6].

The method employed for the determination of L-shell ionization probabilities is based on the observation of Kα X-ray satellites. Using high resolution crystal spectrometers we were able to separate the diagram and the satellite Kα X-ray lines corresponding to "spectator" L-shell holes present at the time of the X-ray transition. From the satellite line yield distribution the L-shell ionization probabilities in near central collisions were determined. In this method, the selection of small (in the L-shell scale) impact parameters is automatically ascertained by the requirement of simultaneous K and L shell ionization. The experimental details and examples of the observed spectra have been presented earlier [1–6]. The data were analyzed by fitting the sum of the Voigt profiles resulting from the convolution of the natural (*i.e.* Lorentzian) line shape with the Gaussian instrumental response function. The multiplet structure of the L satellites arising from the angular momentum coupling of the open shells and the influence of additional M-shell ionization is approximated by treating the positions and instrumental line widths as adjustable parameters.

The experimental satellite line yield distribution corresponds to the vacancy distribution at the moment of the K X-ray transition. It may differ from the initial vacancy distribution because of several possible processes (the Auger and radiative transitions), leading to the filling of the L-shell holes prior to the Kα X-ray emission. These redistribution effects have been corrected for by using a statistical scaling procedure [1].

The average L-shell ionization probabilities were determined from the least squares fit of the binomial distribution to the primary vacancy distribution. This method is essentially based on the assumption that all electrons are ejected simultaneously in an uncorrelated way. For not too large DI and EC ionization probabilities ($p_{\rm L}^{\rm DI}$ and $p_{\rm L}^{\rm EC}$) the primary vacancy distribution can be described in the first approximation by a binomial distribution with the average L shell ionization probability $p_L = p_L^{DI} + p_L^{EC}$ as a free parameter. Small deviations from the binomial statistics might be expected due to the fact that the binding energies of the L-shell electrons increase with the degree of L-shell ionization, and the vacancy distribution following EC to the K-shell of the projectile is governed by the limiting constraint of having only two K-shell vacancies available [1].

The experimental results are compared with theoretical CTMC [7] and SCA-HYD calculations [8]. The SCA-HYD method is based on the first order perturbation theory and the independent particle picture. The projectile motion is described classically allowing the impact parameter dependent formulation of the direct Coulomb ionization probabilities. In the calculations reported here, screened relativistic hydrogenic-like wave functions are used for the description of the bound electron states. According to [3–6, 9], such an approximation of the atomic target wavefunctions is rather crude, and for collision velocities exceeding the orbital velocity of the ionized electrons it leads to systematic disagreement with the experimental inner-shell ionization probabilities. In the CTMC approach exact three-body classical equations of motion are solved for trajectories whose initial conditions are chosen from the microcanonical ensemble. One of the merits of the CTMC method is that it provides both the DI and EC impact parameter dependent inner shell ionization probabilities.

TABLE I

Summary of experimental and theoretical L-shell ionization probabilities (per electron) for $_{42}$Mo, $_{46}$Pd, (see Ref. [1]); $_{57}$La, $_{73}$Ta, $_{92}$U, (Refs [3–6]); and $_{60}$Nd, $_{65}$Tb, (Ref. [2]) targets bombarded by ^{14}N, ^{16}0, and ^{20}Ne ion beams.

System	η_L	Experimental probability[%]	Theoretical probability[%] SCA-HYD	Theoretical probability[%] CTMC Total	D.I.	E.C.
500 MeV Ne + U	0.844	4.8(1.2)	3.13	4.66(16)	3.71(14)	0.96(7)
86.4 MeV O + Pd	0.945	10.2(7)	9.17	11.56(25)	8.50(21)	3.05(13)
300 MeV Ne + Tb	1.004	8.84(37)	5.91	8.32(13)	6.56(12)	1.77(6)
210 MeV N + Tb	1.004	4.75(39)	2.85	4.22(15)	3.46(13)	0.76(6)
88 MeV O + Mo	1.071	12.5(9)	10.2	12.45(26)	9.48(23)	2.97(12)
210 MeV N + Nd	1.110	5.00(40)	3.08	4.82(16)	4.01(14)	0.82(6)
350 MeV N + Ta	1.135	3.31(28)	2.00	3.16(13)	2.81(12)	0.35(4)
403 MeV N + La	1.653	3.31(14)	1.97	3.35(13)	3.08(13)	0.26(4)

The results of the SCA-HYD and CTMC calculations and the experimental average L-shell ionization probabilities are listed in Table I. The CTMC results are given for the DI process alone as well as for the sum of DI plus EC contributions. In Fig. 1 the ratio between the experimental and theoretical L-shell ionization probabilities is plotted as a function of the reduced velocity η_L, *i.e.* the ratio between the projectile velocity and the average "Bohr" velocity of the target L-shell electrons. Such a representation of the experimental data allows to investigate the overall features of the SCA-HYD and CTMC models. These features are shortly summarized below.

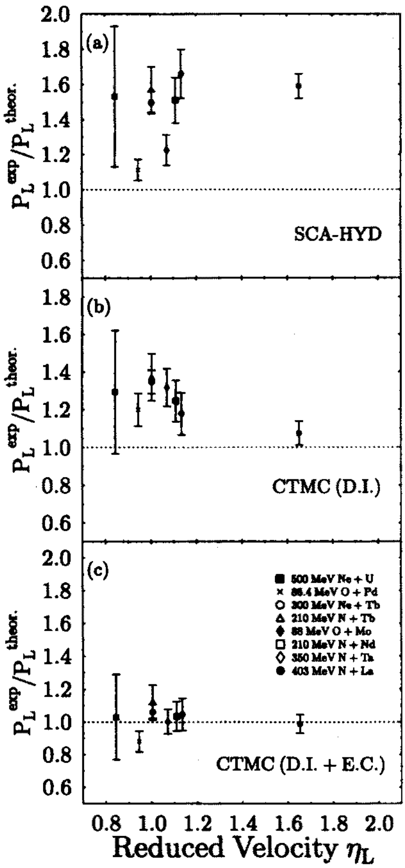

Fig. 1. Ratio of the experimental to theoretical L-shell ionization probabilities in three models: (a) SCA-HYD with screened hydrogenic-like wavefunctions, (b) CTMC [7] calculations of DI ionization probabilities, (c) CTMC calculations taking into account DI and EC mechanisms of ionization.

The SCA-HYD calculations using screened hydrogenic-like wavefunctions (see Fig. 1(a)) systematically underestimate the experimental data. Part of the observed discrepancies can be explained by the EC process which is not included in the SCA-HYD model. However, the electron capture is expected to play an important role only in the narrow region where $\eta_L \simeq 1$. For reduced velocities $\eta_L > 1$ the inaccuracy of the SCA-HYD theory can be thus associated with the inadequate (hydrogenic-like) wavefunctions used in these calculations [5, 6, 9]. It has been shown recently, that the use of more realistic potentials for the determination of the atomic target wavefunctions substantially reduce the discrepancies found for L- and M-shell ionization with hydrogenic-like models. It has been demonstrated, that especially for fast collisions the SCA calculations with variationally determined and optimized wavefunctions [5, 6], or fully self consistent field Hartree–Dirac–Fock wavefunctions [10] yield an almost quantitative agreement with the experimental data. It would be desirable to perform those calculations for the whole range of bombarding energies and ions studied here.

In Fig. 1(b) the experimental L-shell ionization probabilities are compared with CTMC calculations taking into account only the DI process. The excess of experimental p_L values observed for $\eta_L \simeq 1$ can be interpreted as a result of non-negligible contribution of the electron capture process. For reduced velocities η_L substantially larger than 1 (*e.g.* in the case of 403 MeV N + La), where the EC is expected to play a minor role, the CTMC (DI) calculations are in much better agreement with the experimental data than the SCA-HYD results.

A very good absolute agreement is obtained between the experimental data and the CTMC calculations if both the EC and DI mechanisms of ionization are taken into account Fig. 1(c). This somewhat surprising result can be explained using the arguments of C. Reinhold *et al.* [11]. These authors showed that for large momentum transfers, *i.e.* for ionization at small impact parameters, and not too high collision energies, the quantal results converge to classical ones.

Due to its non-perturbative nature, the CTMC approach has been applied in the past mainly to the strongly coupled ion–light atom collisions yielding in general a good agreement with the experimental multiple ionization cross sections. Only few studies were devoted to the investigation of the applicability of CTMC method for the description of inner shell ionization probabilities for small impact parameters. Sharabati *et al.* [12] have measured the $p_L(b)$ for collisions of 0.5 and 1.0 MeV protons with neon atoms in the impact parameter regime $b \leq r_K$, where r_K is the expectation value for the Ne K-shell radius. They found that the CTMC calculations are in good agreement with the experimentally determined $p_L(b)$. We have shown in the present paper that the CTMC calculations are also capable to predict accurately the L-shell ionization probabilities in near central collisions with mid-Z and heavy atoms for η_L in vicinity of one, where both DI and EC processes play an important role.

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