Relativistic calculations of inner-shell atomic processes in low-energy ion-atom collisions*

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In the recent work [1] we developed a relativistic method for evaluation of charge-transfer and electron-excitation processes in low-energy ion-atom collisions. Here we report on a recent application of this method for the evaluation of K-shell-vacancy production and K-K-shell charge transfer probabilities versus the impact parameters in low-energy collisions of H-like ions with neutral atoms. The calculations are performed for systems already studied experimentally and theoretically [2, 3, 4, 5], as well as for systems, which will be investigated experimentally at GSI and FAIR (Darmstadt) in the near future [6].

The method of calculations is based on the independent particle model, where the many-particle Hamiltonian $\hat{H}$ is approximated by a sum of effective single-particle Hamiltonians $\hat{H}^{\rm eff} = \sum \hat{h}^{\rm eff}$ reducing the electron many-particle problem to a set of single-particle equations. The latter is solved by means of the coupled-channel approach with atomic-like Dirac-Fock-Sturm orbitals [1], localized at the ions (atoms). The solutions of these equations allow one to describe the many-electron collision dynamics. The Dirac-Kohn-Sham Hamiltonians with the exchange-correlation potential taken in the Perdew-Zunger parametrization [7] are used as effective single-particle Hamiltonians.

In our calculations the projectile (H-like ion) moves along a straight line with a constant velocity and the target (neutral atom) is fixed. Only the $1s$ electron of the target is considered as the active electron and participates in excitation and charge-transfer processes, while the electrons of the target provide a screening potential. In Fig. 1 we present the results of the calculations for the Ne – $F^{8+}(1s)$ collision at the projectile energy 525 keV/u. We note that the K-shell-vacancy production is mainly determined by the K-K-shell charge transfer. At small impact parameters the contribution from the charge-transfer excitation into the $2s$, $2p$, and higher vacant states of the projectile become also important. The related calculations of the K-shell-vacancy production are performed for the Xe – $Xe^{53+}(1s)$ collision at the projectile energy of 5.9 MeV/u in the relativistic and nonrelativistic limits. As one can see from Fig. 2 the role of the relativistic effects is rather strong. We note that both curves have the same oscillatory behavior but the nonrelativistic curve is shifted toward larger impact parameters.

In our further investigation we plan to continue investigation of inner-shell electron processes in low-energy ion-atom collisions. Special attention will be paid to the many-particle effects.

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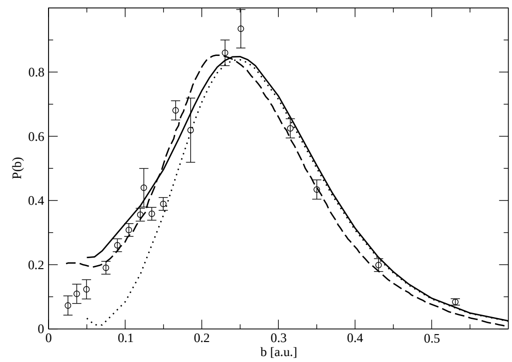

Figure 1: The probabilities $P(b)$ of the Ne K-shell-vacancy production (solid line) and of the K-K-shell charge transfer (dotted line) as functions of the impact parameter b for the Ne-$F^{8+}(1s)$ collision at the projectile (fluorine) energy of 525 keV/u. The circles indicate experimental results by Hagmann *et al.* [2]. The dashed line presents theoretical results by Fritsch and Lin [3].

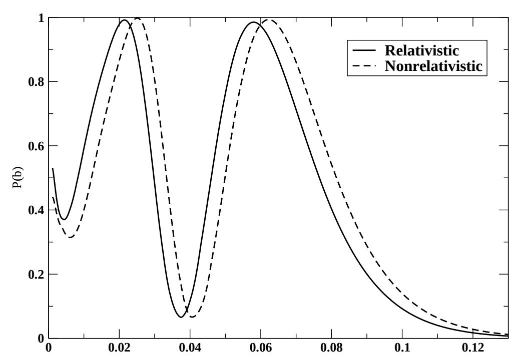

Figure 2: The probability $P(b)$ of the Xe K-shell-vacancy production in the Xe-$Xe^{53+}(1s)$ collision as a function of the impact parameter b at the projectile energy of 5.9 MeV/u.

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