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Multiple electron transfer in slow collisions of highly charged ions and atoms

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Abstract

Multi-electron transfer processes in slow collisions $Ar^{q+} + Ar$ ($q = 5, \ldots, 10$) have been studied theoretically by means of a molecular dynamics approach. We discuss the electron transfer dynamics, in particular with respect to the assumptions made in overbarrier models. Furthermore, absolute cross-sections are defined and compared to experimental data.

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1. Introduction

Collisions of slow highly charged ions with multi-electron target atoms have been extensively studied experimentally for more than two decades by now, see e.g. [1–4]. The dominant process at low velocities, i.e. $v < 1$ au (atomic unit), is multiple electron transfer. The interpretation of the physical mechanisms as well as the calculation of measurable quantities like cross-sections was done almost exclusively in terms of so-called classical overbarrier models [4,5]. The first formulation for multi-electron processes by Bárány [4] was followed by the more sophisticated model by Niehaus [5]. Despite of their simplicity, these overbarrier models have been surprisingly successful in analyzing experimental data [3–5]. However, they require the appropriate definition of critical radii, screening charges, and capture probabilities. Here we present dynamical calculations where we do not have to define these quantities a priori, but instead they can be deduced from the calculations. We present applications to collisions of argon where absolute measurements of total as well as one- and two-electron transfer cross-sections have been reported [1–3].

2. Theoretical model

To simulate the collision process we use classical molecular dynamics (MD). Initially, electrons bound to the target atom are not treated explicitly, rather they are created through the course of the collision. Therefore we calculate the potential which the most weakly bound target electron would see if it would have been created. This is

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done along the line connecting the target at $\vec{R}_t$ with charge Q_t (for the 1st electron $Q_t = 1$, for the 2nd $Q_t = 2$ and so on) and the projectile at $\vec{R}_p$ with charge Q_p, i.e. $\vec{r}_\lambda = \vec{R}_t + \lambda(\vec{R}_p - \vec{R}_t)$ with λ a parameter between 0 and 1. The potential reads

$$V(\vec{r}_\lambda) = -Q_t W(\vec{r}_\lambda - \vec{R}_t) - Q_p W(\vec{r}_\lambda - \vec{R}_p) + \sum_{i=1}^{n} W(\vec{r}_\lambda - \vec{r}_i), \quad (1)$$

with the form of the interaction potential W defined below (cf. Eq. (2)). There are n electrons created so far and located at $\vec{r}_i$. (Initially $n = 0$) With the potential (1) and the (Stark-shifted [1]) binding energy E_b we decide at every timestep Δt whether the most weakly bound electron of the target is released or not. For that we used two different criteria:

Overbarrier ionization (OBI). If $E_b \geqslant \max V(\vec{r}_\lambda)$ a previously bound electron is placed at the top of the barrier. This is similar to the transfer mechanism assumed in the overbarrier models.

Tunnel ionization (TI). We calculate the tunnel rate [6]

$$\Gamma = \frac{1}{T_b} \exp\left(-2 \int_{\lambda_1}^{\lambda_2} d\lambda \sqrt{2[V(\vec{r}_\lambda) - E_b]} \right),$$

with T_b the classical period of the bound electron and $\lambda_{1,2}$ the classical turning points defined by $V(\vec{r}_{\lambda_{1,2}}) = E_b$. The tunnel probability over a time interval Δt is given by the product $\Gamma \cdot \Delta t$. If this probability is greater than a random number (between 0 and 1) the electron is placed at $\vec{r}_{\lambda_2}$, i.e. on the line connecting target and projectile at the outerside of the barrier. This mechanism is of great importance for the ionization of atoms or clusters by intense laser pulses [7].

Once the electrons are created they are propagated in the Coulomb field of all the other particles. A standard propagation scheme with a fixed time step of $\Delta t = 2.4 \times 10^{-18}$ s resulted in errors of the energy conservation less than 0.1 eV. We use a softened Coulomb potential between two particles at a distance r:

$$W(r) = \begin{cases} \frac{1}{2a}\left[3 - \left(\frac{r}{a}\right)^2\right] & r \leqslant a, \\ \frac{1}{r} & r > a, \end{cases} \quad (2)$$

with $a = 2.5$. Such softening prevents the unphysical instability of classical simulations with bare Coulomb interaction and is routinely used in applications to laser-atom interaction [7].

3. Results and discussion

In what follows we present studies of collisions

$$Ar^{q+} + Ar \rightarrow Ar^{(q-m)+} + Ar^{k+} + (k-m)e^-,$$

with a fixed impact velocity of $v = 0.22$ au. First we will discuss as a typical example the collision dynamics of $Ar^{5+} + Ar$. Fig. 1 shows the time evolution of the target and projectile charges for a particular collision event with an impact parameter $b = 5$ au. The three electrons created are of molecular character (cf. the strong charge oscillation around $z \sim 0$) and may finally be captured by either the target or the projectile (cf. the diminishing oscillations for larger z).

Fig. 2 shows for the same collision system the removal probabilities for the 1st and 2nd electrons

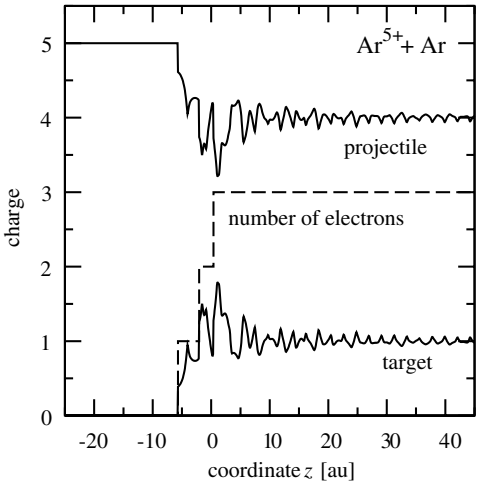

Fig. 1. Projectile and target charges as a function of z, the coordinate of the projectile along its trajectory, for a typical simulation of an Ar^{5+} ($v = 0.22$ au) + Ar collision (impact parameter $b = 5$ au). The target is initially at $z = 0$. The actual number n of 'molecular' electrons is shown as well.

[1] This shift is given by the field of the projectile and of all n so far created electrons.

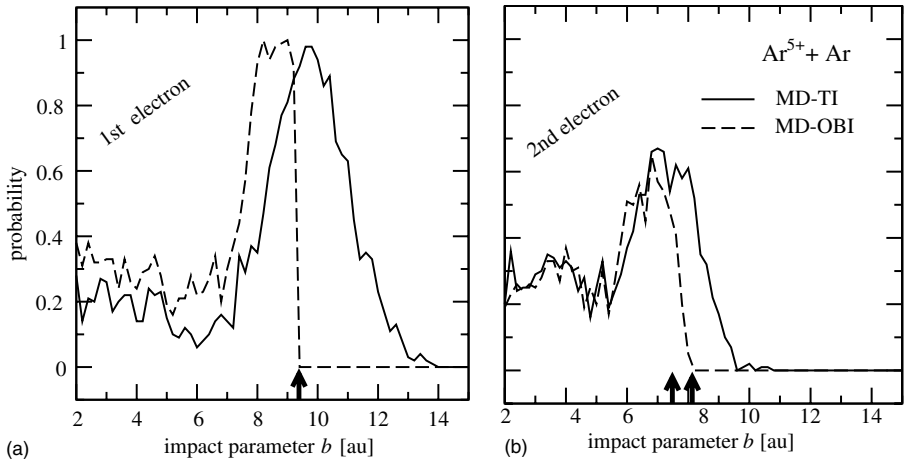

Fig. 2. Removal probability of the 1st and 2nd electron as a function of the impact parameter for the two ionization criteria discussed in the text. The arrows mark the critical radii from the overbarrier models of Bárány [4] and Niehaus [5]. Whereas they are equal for the 1st electron, Niehaus obtains a larger one for the 2nd electron.

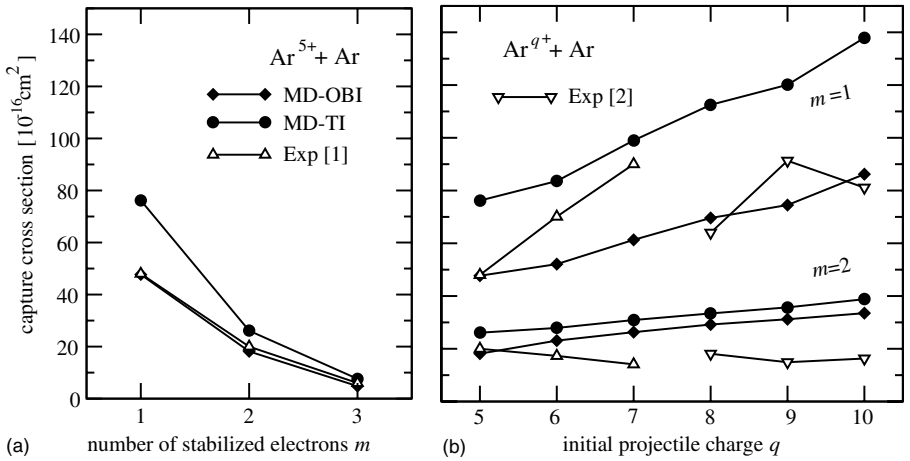

Fig. 3. Cross-sections for collisions $Ar^{q+} + Ar \rightarrow Ar^{(q-m)+} + Ar^{k+} + (k-m)e^-$ at $v = 0.22$ au. The present work is compared with experimental data. Left panel: $q = 5$ and $m = 1, 2, 3$. Right panel: $q = 5, \ldots, 10$ and $m = 1$ and $m = 2$.

as a function of the impact parameter. Each point represents an ensemble average of 100 collisions. [2] For the first electron removed from the target (shown in the left panel of Fig. 2) there is a large difference for the two criteria of target ionization introduced above. Whereas the OBI posses a strong increase at the critical radius of the over-barrier model the TI approach leads to transfer at considerably larger impact parameters. In both cases the removal probability for impact parameters below the highest one is close to 100%. One should note that for smaller impact parameters ($b \leqslant 7$ au) there is still a remarkable probability (10–30%) which is, however, less important for the

[2] Note that single trajectories of such an ensemble are different due to the random numbers entering the electron creation despite their identical initial conditions. The ensemble average, however, is independent on these random numbers.

cross-section. For the 2nd electron transferred the situation is different as it is influenced by the already existing electron. We emphasize that this applies not only for the dynamics but also for the creation process. As can be seen in the right panel of Fig. 2 the difference between OBI and TI is less pronounced and the maximal value of the probability is only about 60%. It is interesting to note that the appearance of a finite probability coincides quite well with the radius assumed in the Niehaus model [5].

Whereas the removal probability is exclusively defined by the transfer process, the number of stabilized electrons at the target is additionally influenced by the decay of the 'hollow' projectile. This decay occurs by fast autoionization processes which are to some extent contained in our dynamical simulation. We found by comparing our decay probabilities with those obtained from experimental cross-sections [8] that the propagation of the electron dynamics to about 0.2 ps after the collision is sufficient. Fig. 3 shows absolute cross-section for different numbers m of stabilized electrons. Whereas the OBI approach for $Ar^{5+} + Ar$ (cf. left panel of Fig. 3) agrees almost perfectly with the experiment independently on m, TI typically overestimates the cross-sections. This may be caused by the effect that allowing tunneling for transfer from the target to the projectile favours this direction. For higher projectile charges we find a monotonic increase of the cross-sections (cf. right panel of Fig. 3). The slightly higher slope in our work may be caused by omitted decay processes, e.g. radiative decay.

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