Ionization and electron capture processes induced in collisions between singly charged ions and nitrogen atom

M. Al-Ajaleen[1,2], A. Taoutioui[1], K. Tőkési[1]

[1] *Institute for Nuclear Research (ATOMKI), Debrecen, Hungary*

[2] *Doctoral School of Physics, University of Debrecen, Debrecen, Hungary*

Introduction

The inelastic electron processes induced in ion-atom collisions are crucial and central in numerous research domains such as modelling and diagnosing fusion plasma in tokamak reactors and interstellar space [1, 2]. The control of these processes rely on the accurate cross-sections of the induced electron processes. In this work, our main interest is to present an accurate total cross-sections for single-electron processes, mainly single-electron capture and single ionization in collisions between singly charged ions and ground-state nitrogen atoms. Since we are interested in single-electron processes, the collision system can be considered as a three-body problem in which the nitrogen target is described within the single active electron approximation (SAE) using a model potential where only the outermost electron is involved in the collision dynamics [3]. The scattering problem is solved within the frame of the classical trajectory Monte Carlo (CTMC) [4].

Theoretical Model

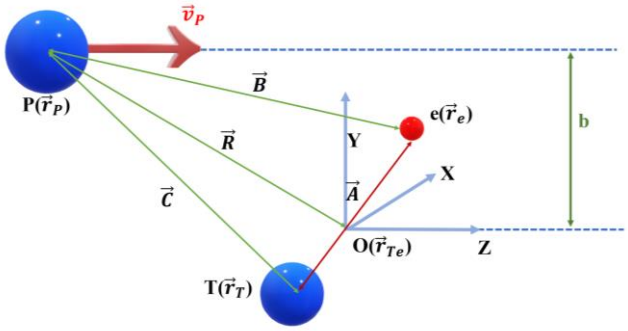

Figure 1: The schematic diagram of the three-body collision system. $\vec{A}$, $\vec{B}$ and $\vec{C}$ are the position vectors of the interacting particles, $\vec{R}$ is the distance between projectile and the centre of mass of the target-electron, b is the impact parameter.

The Li^+-*N(2p)* collision system is reduced to a three-body system. The three bodies are the followings: the projectile (P), the target core (T) and the active target electron (e) (see figure 1). In our calculations we used the model potential developed by Green [6] to describe the interaction between the particles. The model potential can be written as:

$$V(r) = q\frac{Z-(N-1)\big(1-\Omega(r)\big)}{r} = q\frac{Z(r)}{r} \tag{1}$$

where Z and N are the nuclear charge and number of electrons respectively, *r* is the distance between test charge q and Z, and Ω(r) is the screening potential having the form:

$$\Omega(r) = \left[(\eta/\xi)\left(e^{\xi r}-1\right)+1\right]^{-1}. \tag{2}$$

We note here, that the potential has a correct asymptotic form for both small and large values of *r* which are stated as follow:

At large interaction distance *r*, $\lim_{r\to\infty}\Omega(r) = 0$, hence the N electrons are included in the model potential, however, at close interaction, $\lim_{r\to 0}\Omega(r) = 1$. In this case, only the nuclear charge Z contributes to the model potential. The parameters η and ξ for the projectile P and target T are expressed as:

$$\eta_P = \eta_P^{(0)} + \eta_P^{(1)}(Z_P - N_P - 1) \tag{3}$$

$$\xi_P = \xi_P^{(0)} + \xi_P^{(1)}(Z_P - N_P - 1) \tag{4}$$

$$\eta_T = \eta_T^{(0)} + \eta_T^{(1)}(Z_T - N_T) \tag{5}$$

$$\xi_T = \xi_T^{(0)} + \xi_T^{(1)}(Z_T - N_T) \tag{6}$$

Equations 3-6, and the values of the parameters $\eta_X^{(0)}, \eta_X^{(1)}, \xi_X^{(0)}, \xi_X^{(1)}$ (X=T or P) are tabulated by Garvey *et al* [3]. The total potential energy, *V* and the Hamiltonian, *H* of our three-body system can be written as:

$$V(A,B,C) = \frac{Z_P(C)Z_T(C)}{C} - \frac{Z_T(A)}{A} - \frac{Z_p(B)}{B} \tag{7}$$

$$H = \frac{P_P^2}{2m_P} + \frac{P_T^2}{2m_T} + \frac{P_e^2}{2m_e} + V(A,B,C) \quad (8)$$

where *m*, Z are the mass, the charge for the labelled particles, and *A,B,C* are the relative distances among the corresponding particles. From the associated canonical equations, we get 12 coupled first-order differential equations. These equations are solved in the CTMC simulation using the 4th order Runge-Kutta method. Calculating the total cross section requires a considerable number of trajectories to reduce the statistical uncertainty as low as possible. The total cross section of a certain process σ, and the associated statistical uncertainty are given by the following formulas:

$$\sigma = \frac{2\pi b_{max}}{N} \sum_j b_j. \quad (9)$$

$$\Delta\sigma = \sigma \left(\frac{N - N_P}{N N_P}\right)^{1/2}. \quad (10)$$

where *N* is the total number of trajectories calculated in the impact parameter range between 0-b_{max} and N_p is the number trajectories that satisfy the criteria of the given exit channel.

Results

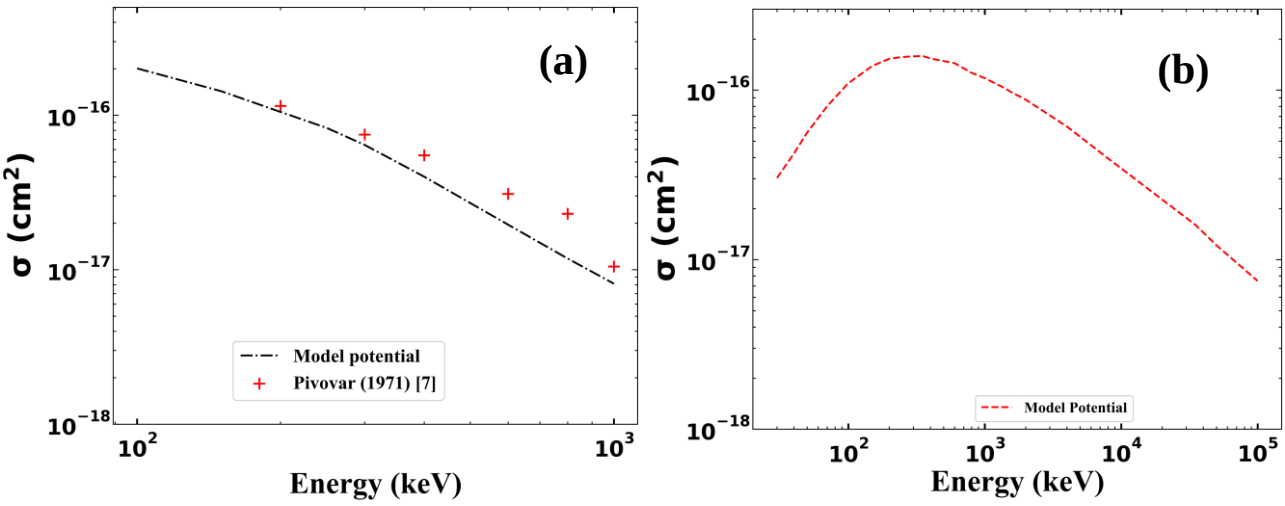

Figure 2: Total cross-section of the single electron processes in Li^+-*N(2p)*. **a**) single electron charge exchange cross sections **b**) single target ionization cross sections.

Figure 2 shows the total cross-sections of single capture and single target ionization in Li^+-*N(2p)* collisions obtained by CTMC method. Figure 2a shows the single electron charge exchange cross sections as function of the projectile impact energy from 100 keV to 1 MeV. We found that our CTMC results are in a good agreement with the experimental results of Pivovar [7]. Due to lack of previous data, figure 2b shows our CTMC results for the single ionization cross sections as function of the projectile impact energy in the range between 10 keV and 100 MeV. From the figure we can notice that the maximum of the ionization total cross-section is around 300 keV. At projectile impact energies greater than 5 MeV the ionization cross-section decrease dramatically.

Summary

We have presented classical trajectory Monte Carlo calculations of single electron charge exchange and ionization cross-section in collision between single charged Li ion and Nitrogen atom. We found that our classical results are in good agreement with the available experimental data.

Acknowledgements This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

References

1. R. Isler et. al., *Nucl. Fusion*, **31** (1991) 245–25.
2. R. Hemsworth et. al., *Nucl. Fusion*, **49** (2009) 045006.
3. R. H. Garvey et. al., *Phys. Rev. A*, **12** (1975) 1144–1152.
4. K. Tökési and G. Hock, *Nucl. Instrum. Methods Phys. Res. B: Beam Interact. Mater. At.*, **86** (1994) 201–204.
5. A. Harris, *atoms*, **7** (2019) 44.
6. A. Green, *Adv. Quantum Chem.*, **7** (1973) 221–262.
7. L. Pivovar et. al., *Sov. Phys. JETP*, **32** (1971) 19–28.