Publ. Astron. Obs. Belgrade No. 84 (2008), 161 - 164 *Contributed Paper*

NEUTRALIZATION DISTANCES OF Ar^{Z+} RYDBERG IONS INTERACTING WITH SOLID SURFACES

M. D. MAJKIĆ, N. N. NEDELJKOVIĆ and S. M. D. GALIJAŠ

Faculty of Physics, University of Belgrade, P.O.Box 368, Belgrade, Serbia
E–mail: hekata@ff.bg.ac.yu

Abstract. We apply the recently developed time-symmetrized, two-state vector model to investigate the intermediate stages of the electron capture into the Rydberg states of multiply charged Ar^{Z+} ions (core charge $Z \gg 1$, principal quantum number $n_A \gg 1$) escaping Al-solid surface at low velocity. The simple analytical formulae derived for the corresponding neutralization rates enable us to analyze the neutralization distances for the low-l Rydberg states (n_A, l_A, m_A), for different charge states Z of the ion. It is found that the inclusion of core polarization significantly reduces the neutralization distances. The neutralization distances for the highest Rydberg levels that can be populated in the vicinity of solid surface are in agreement with the data deduced from experiments in which the kinetic energy gain due to the image acceleration of the ions is measured.

1. INTRODUCTION

The electron exchange during the interaction of ions with solid surfaces has been intensively studied both theoretically and experimentally; see, e.g. Reviews by Burgdorfer (1993) and Winter (2002). However, the quantum description of the events in the time interval between the initial and final "measurements" is still uncompleted. Recently, this kind of problem has been considered within the framework of two-state vector model (TVM) by Nedeljković and Nedeljković (2007), concerning the neutralization dynamics of the multiply charged ions in the interaction with solid surfaces. The model has been adapted to the intermediate stages of the population dynamics and to the low-velocity regime.

The TVM represents a form of the time-symmetric formulation of quantum mechanics; namely, the state of a single electron is described by two state vectors $|\Psi_1(t)\rangle$ and $|\Psi_2(t)\rangle$. The first state evolves from the initial state $|\Psi_1(t_{in})\rangle$ towards the future, while the second state evolves "teleologically" towards the fixed final state $|\Psi_2(t_{fin})\rangle$ detected in the final time $t = t_{fin}$. The TVM has been applied to the ions ArVIII, KrVIII and XeVIII (all with core charges $Z = 8$), and to the ions SVI, ClVII and ArVIII (with core charges $Z = 6, 7$ and 8, respectively), see e.g. Nedeljković and Nedeljković (2007) and Nedeljković et al. (2008).

In the present paper, we analyze the electron capture (neutralization) into the Rydberg states of multiply charged Rydberg ions escaping solid surfaces at low velocity, considering the ions Ar^{Z+} for $Z = 5 - 10$. We use the simple analytical expressions

for the probabilities and rates obtained by Nedeljković and Nedeljković (2007) to calculate the neutralization distances R_c^N, for the ions finally detected in the spherical Rydberg state $\nu_A = (n_A, l_A, m_A)$ with principal quantum number $n_A \gg 1$, low values of the orbital quantum number l_A, and $m_A = 0$. In the applied TVM treatment of intermediate stages of neutralization, the polarization of the solid, as well as the polarization of the electronic cloud of the ionic core are taken into account. The neutralization distances R_c^N for the particular (critical) Rydberg state $n_A = n_{max}$ can be compared with the values deduced from the measured projectile kinetic energy gains in the step-wise neutralization under grazing incidence, see e.g. Winter (1992) and Winter et al. (1993).

2. NEUTRALIZATION DISTANCES IN TVM

Within the framework of the TVM, the neutralization distances R_c^N are defined via the intermediate neutralization probabilities $P_{\nu_A}(t)$. That is, we use the normalized probability $\tilde{P}_{\nu_A}(t) = P_{\nu_A}/P_{\nu_A}^{fin}$, and the corresponding rate $\tilde{\Gamma}_{\nu_A}(t)$. By definition, the quantity $\tilde{P}_{\nu_A}(t)$ represents the neutralization probability at the time t under the condition that the state $|\nu_A\rangle$ is populated at the time $t \to t_{fin}$ with certain. We note that the TVM is almost independent of the form of the near-surface potential, and a dynamical response of the surface can be neglected, so that the classical electrostatic image potentials can be used outside the surface. The interaction of the active electron with polarized ionic core can be represented by the Simons-Bloch potential, which accounts for the experimentally observed quantum defects of the ionic energy spectra.

Under these conditions we get the following expressions for the probability $\tilde{P}_{\nu_A}(t)$ and the corresponding rate $\tilde{\Gamma}_{\nu_A}(t)$, see e.g. Nedeljković and Nedeljković (2007):

$$\tilde{P}_{\nu_A}(t) = \left[1 - \left(\frac{R}{R_{in}^*}\right)^{\tilde{\alpha}} \mathrm{e}^{-\tilde{\beta}(R-R_{in}^*)}\right]^2, \tag{1}$$

$$\tilde{\Gamma}_{\nu_A}(t) = 2v\left(\frac{R}{R_{in}^*}\right)^{\tilde{\alpha}}\left(\frac{\tilde{\alpha}}{R} - \tilde{\beta}\right)\mathrm{e}^{-\tilde{\beta}(R-R_{in}^*)}\left[\left(\frac{R}{R_{in}^*}\right)^{\tilde{\alpha}} \mathrm{e}^{-\tilde{\beta}(R-R_{in}^*)} - 1\right]. \tag{2}$$

In the above equations we have $\tilde{\beta} = (\gamma_M + \tilde{\gamma}_A)/2$ and $\tilde{\alpha} = Z/\tilde{\gamma}_A - 1/2 + 1/4\gamma_M$, where $\gamma_M = \gamma_A(R)$; by $\tilde{\gamma}_A$ we denoted the energy parameter of the active electron in the field of polarized ionic core, and $\gamma_A = \tilde{\gamma}_A + (2Z-1)/4R$ is the corresponding energy parameter shifted due to the interaction with polarized solid. The quantity R_{in}^* is the minimal ion-surface distance at which the resonant neutralization is allowed.

The rates $\tilde{\Gamma}_{\nu_A}(t)$, are directly related with the problem of localization of the neutralization process. That is, the maxima of the rates $\tilde{\Gamma}_{\nu_A}(t)$ determine the neutralization distances R_c^N for the process $A^{Z+} + M(e) \to A^{(Z-1)+} + M$, i.e.,

$$\left(\frac{d\tilde{\Gamma}_{\nu_A}(t)}{dt}\right)_{R=R_c^N} = 0. \tag{3}$$

We point out that the neutralization distances defined within the framework of the TVM are related to the fraction of ions with a given final state $\nu_A = (n_A, l_A, m_A)$, but with an arbitrary initial states μ_M, thus the neutralization distances R_c^N depend only on n_A and l_A (for $m_A = 0$).

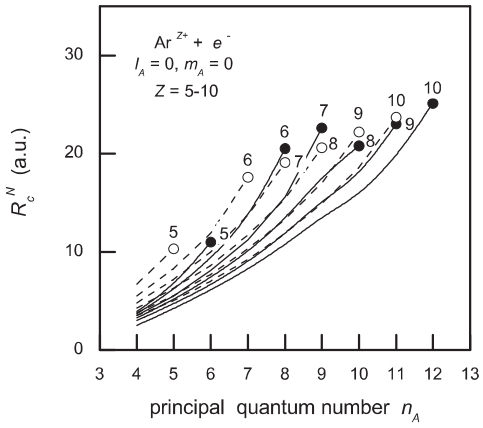

Figure 1: Neutralization distances R_c^N of the ion Ar^{Z+} interacting with Al surface, for the electron capture into the Rydberg states $n_A \leq n_{max}$, $l_A = 0$, $m_A = 0$. Dashed curves correspond to the point-like core case. The quantum numbers n_{max} are marked by dots and circles, for the polarized and non-polarized ionic cores, respectively.

3. RESULTS

We apply the expression (3) to calculate the neutralization distances for the Ar^{Z+} ions with core charges $Z \in [5, 10]$. We consider the Rydberg states (n_A, l_A, m_A) for $n_A \leq n_{max}$ where n_{max}, represents the quantum number n_A of the highest level that can be populated; for the angular momentum quantum number l_A and the quantum number m_A we take the value $l_A = m_A = 0$.

The maximal value of the principal quantum number corresponds to the Rydberg state populated from the vicinity of the Fermi level. Within the framework of the TVM, the quantity n_{max} is defined by the condition: $\gamma_{max}(R_c^N) = \gamma_\phi + \delta\gamma$, where $\gamma_{max}(R)$ is the energy parameter of the active electron in the first scenario (conduction band energy parameter), which gives the main contribution to the population of the considered state, γ_ϕ is the energy parameter of the Fermi level and $\delta\gamma$ is the mean distance between the energy terms. In the low-velocity case considered in the present paper we have the quasi-resonant condition $\gamma_{max}(R) \approx \gamma_A(R)$.

In Fig. 1 we present (full curves) the neutralization distances R_c^N via principal quantum number n_A, for the Ar^{Z+} ion interacting with Al solid surface with work function $\phi = 5$ eV. Dashed curves in Fig. 1 are the neutralization distances obtained in the point-like core case. From Fig. 1 we recognize that the polarization of the ionic cores plays an important role in the considered low-l_A case; the neutralization distances are significantly overestimated if the polarization is neglected. The neutralization distances for the electron capture into the critical Rydberg states with $n_A = n_{max}$ are marked by dots and circles, for the polarized and the point-like core charges Z, respectively. It is intriguing that the R_c^N-curves obtained for the polarized ionic cores with a core charge Z nearly coincide with the curves related to the non-polarized core cases, for the core charges $Z + 1$.

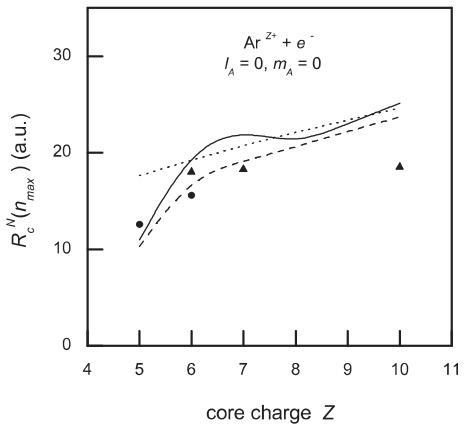

Figure 2: Neutralization distances R_c^N for $n_A = n_{max}$ and $l_A = 0$ of the ion Ar^{Z+} interacting with Al surface. Dashed curve corresponds to the point-like core case. Symbols are the experimental data, see e.g. Winter (1992) and Winter et al. (1993). By dotted line we presented the COB-neutralization distances R_c^{class}.

At present, the experimental evidence of the intermediate stages of the neutralization process of the considered Ar^{Z+} ions exists only for the projectiles impinging the surface under grazing geometry, and only for $n_A = n_{max}$. The corresponding neutralization distances R_c^N can be deduced from the measured projectile kinetic energy gains $\Delta E = Z^2/4R_c^N$, see e.g. Winter (1992) and Winter et al. (1993). In Fig. 2 we present the neutralization distances R_c^N for $n_A = n_{max}$ and $l_A = m_A = 0$ of the ion Ar^{Z+} interacting with Al surface, together with the experimental data for Ar^{Z+} (dots, Winter 1992) and Xe^{Z+} (triangles, Winter et al. 1993). In Fig. 2 we also present the first neutralization distance $R_c^{class} = \sqrt{8Z+2}/2\phi$ proposed for $n_A = n_c^{class}$ by COB method, see e.g. Ducrée et al. (1998) and Burgdörfer and Meyer (1993). From Fig. 2 we recognize the agreement of the TVM theoretical predictions with experiment.

To complete the TVM analysis, it is necessary to extend our considerations to other ions and core charges, for example to the case of Xe^{Z+} ions. Also, it remains to include into the TVM the effect of the parallel velocity, which could play an important role in the grazing geometry under which the experiments were performed.

References

Burgdörfer, J.: 1993, Review of Fundamental Processes and Applications of Atoms and Moleculs, eds. C.D. Lin, Singapore: World Scientific.

Burgdörfer, J. and Meyer, F.: 1993, *Phys. Rev. A*, **47**, R20.

Ducrée, J., Casali, F. and Thumm, U.: 1998 *Phys. Rev. A*, **57**, 338.

Nedeljković, N. N. and Majkić, M. D.: 2007, *Phys. Rev. A*, **76**, 042902.

Nedeljković, N. N., Majkić, M. D., Galijaš, S. M. D. and Mitrović, S. B.: 2008, *App. Surf. Sci.*, **10.1016**, j.apsus.2008.05.274.

Winter, H.: 1992, *Europhys. Lett.*, **18**, 207.

Winter, H.: 2002 *Phys. Rep.*, 367 **586**, 387.

Winter, H., Auth, Ch., Schuch, R. and Beebe, E.: 1993, *Phys. Rev. Lett.*, **71**, 1939.