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IONIC VELOCITY AS A MEASURE OF AN INTERPLAY OF THE NEUTRALIZATION ENERGY AND THE DEPOSITED KINETIC ENERGY IN THE SURFACE NANOSTRUCTURE CREATION

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Abstract. We consider the role of the ionic velocity in the nanostructure creation during the interaction of highly charged Xe^{Z+} ions with solid surface.The quasi-resonant two-state vector model and the micro staircase model are used for the analysis of the neutralization process accompanied by the surface modification. For very low ionic velocity, the neutralization energy gives the main contribution in the surface nanostructuring, while for large ionic velocity the nanofeatures are created due to the kinetic energy loss (nuclear and electronic stopping power). The existence of the critical velocity, which separates these two regions, is discussed.

1. INTRODUCTION

In recent years, the highly charged ions (HCI) have been widely used as an effective tool for surface modifications. Depending on the solid type, ionic charge and velocity, different surface nanofeatures can be created, such as craters, hillocks or caldera like structures etc., see Aumayr et al. 2011. For very low ionic velocities ($v < 0.1$a.u.) the surface nanofeatures are created due to deposition of the ionic neutralization energy. For moderate ionic velocities the energy necessary for the nanostructure creation, consists both of the neutralization energy and the deposited kinetic energy (nuclear and electronic stopping power), see Lake et al. 2011 and Majkić et al. 2019.

The aim of the present contribution is to present the role of the ionic velocity in the surface modifications. For that purpose we extend our previous analysis of the HCI neutralization in the interaction with solid surface, see Majkić et al. 2017. We analyze the intermediate Rydberg state population by employing the quasi-resonant

two-state vector model (TVM) and use the micro staircase model for the cascade neutralization.

2. CRITICAL VELOCITY

We consider the HCI of initial charge $Z \gg 1$ impinging upon a metal surface (MV-system) perpendicularly at very low to moderate velocity v. The ionic Rydberg states are populated by the quasi-resonant electron tunnelling through the potential barrier formed between the ion and solid surface. The initial ionic charge $Q = Z$

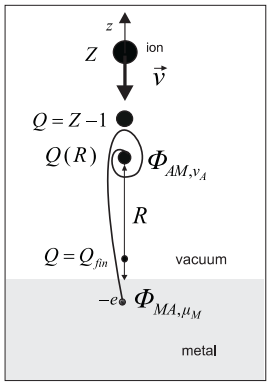

Figure 1: Cascade neutralization of HCI with initial charge Z within the MV-system.

decreases in time, $Q = Q(R)$, approaching the final value $Q = Q_{fin}$ at ion-surface distance $R = R_{min}$ (see Fig. 1). This process is known as cascade neutralization: $Q = Z \to Q = Z - 1 \to ... \to Q_{fin}$; by using the micro-staircase model, we take into account the fine structure of the population process in each macro-cascade. The neutralization process is accompanied by the release of the neutralization energy and its deposition into the surface, which leads to the nanofeatures creation.

Within the framework of the TVM the state of the active electron is described by two wave functions $\Psi_1(\vec{r}, t)$ and $\Psi_2(\vec{r}, t)$, evolving simultaneously in two opposite directions in time: see Nedeljković et al 2007 and Majkić et al. 2019. These functions can be considered as the space-time modifications of the eigenfunctions Φ_{MA,μ_M} and Φ_{AM,ν_A} of the in-Hamiltonian and out-Hamiltonian, respectively, where $\mu_M = (\gamma_M, n_{1M}, m_M)$ and $\nu_A = (n_A, l_A, m_A)$ are the metallic parabolic and atomic spherical quantum numbers, respectively, see Fig. 1. The functions $\Psi_1(\vec{r}, t)$ and $\Psi_2(\vec{r}, t)$ constitute the intermediate two-state of the active electron at the ion-surface distance R, and the corresponding mixed flux $I_{\mu_M,\nu_A}(R)$. The transition probability density is expressed via relation $T_{\mu_M,\nu_A}(t) = \left|\int_R^\infty I_{\mu_M,\nu_A}(R)dR\right|^2 / v^2$; the intermediate Rydberg state population probability is given by $P_{\nu_A}(R) = \int \sum_{n_{1M},m_M} T_{\mu_M,\nu_A}(t)d\gamma_M$. The micro-staircase model for the multielectron neutralization is based on the knowledge of the probabilities $P_{\nu_A}(R)$ and the corresponding neutralization distances. By employing this model we estimate the final ionic charge $Q = Q_{fin}$, see Majkić et al. 2019. The charges Q_{fin} increases with increasing of the ionic velocity v due to the increasing of the population probabilities maxima.

The ion with the initial charge Z (before the neutralization begins) is characterized by the initial potential energy $W_{Z,pot}$. After neutralization cascade, in front of the solid surface at minimal ion-surface distance R_{min}, within the MV-system, the ionic potential energy is given by: $W_{Q_{fin}^{MV},pot}$. The neutralization energy in the considered MV-system is (see Majkić et al. 2019)

$$W^{(Z,MV)} = W_{Z,pot} - W_{Q_{fin}^{MV},pot}. \tag{1}$$

The velocity-behaviour of the neutralization energy is the same as the behaviour of the population probabilities.

For very low ionic velocity, the neutralization process is complete ($Q_{fin} \approx 0$) and the neutralization energy $W^{(Z,MV)} = W_{Z,pot}$ is almost sufficient for the surface nanostructuring. In the case of moderate ionic velocity, due to incompleteness of the neutralization process ($Q_{fin} \neq 0$), both the deposited kinetic energy $E_{k,dep}$ and the neutralization energy $W^{(Z,MV)}$ provide the energy necessary for the nanofeatures formation. These facts indicate the existence of the area of the ionic velocities where the neutralization energy gives the main contribution to the nanofeatures creation, and the complementary one where the kinetic energy loss has to be taken into account. The velocity for which the neutralization and the deposited kinetic energy equally contribute to the nanostructure creation separates these two regions. We denote this value as critical velocity v_c:

$$W^{(Z,MV)}(v_c) = E_{k,dep}(v_c) \tag{2}$$

3. RESULTS

The results obtained in the MV-system we can apply in the analysis of the neutralization process and surface modification in the metal-dielectric-vacuum system (MDV-system) by employing the concept of the effective ionic charge Z_{eff}. That is, we use the expression $W^{(Z,MDV)} = W^{(Z_{eff},MV)}$, see Majkić et al. 2017. It is important to note here that Z_{eff} is a velocity independent quantity.

We analyse the process of the nanocrater formation by impact of slow highly charged Xe^{Z+} ions on the Co surface covered with a thin Al_2O_3 film, see Lake et al. 2011. The experimental values of the ionic velocities are in the region $v \in [0.25, 0.33]$ a.u., so that one expect that both the neutralization energy and the deposited kinetic energy participate in the process of the surface modification. Considering the neutralization cascade in the MDV-system, we take into account that the dielectric film is strongly perturbed during the ionic motion and the process of the nanostructure formation. For that reason we use the value for dielectric constant $\epsilon = 2$ for Al_2O_3 film instead of its optical value $\epsilon = 8$. The corresponding effective ionic charges are calculated in Majkić et al. 2017, and presented in the Table 1.

The kinetic energy $E_{k,dep}$ deposited in the thickness of the film $s_0 = 27$ a.u. are calculated by Lake et al., 2011 for the velocities used in experiment, i.e. for $E_k = 8.1 \cdot Z$ keV. These values can be used to estimate the quantity $E_{k,dep}$ for other velocities assuming the simple proportionality $E_{k,dep} = \kappa E_k$. We get the value $\kappa = 0.03$ for all considered ionic charges $Z \in [25, 45]$. In Fig. 1 we present the neutralization energy and the deposited kinetic energy for the Xe^{Z+} ions within the

Z	25	30	35	40	45
Z_{eff}	18.7	23	27.5	31.4	35
v_c (a.u.)	0.18	0.21	0.23	0.25	0.26

Table 1: Effective core charges Z_{eff} and critical velocities v_c in the case of the crater formation in the MDV-system (Co + Al_2O_3 film) by the impact of Xe^{Z+} ions.

considered MDV-system. The critical velocities v_c are obtained in the intersection of these curves; the corresponding values are presented in Table 1. We note that the calculated values for the critical velocities are in the region of the experimentally used velocity values. This is in accordance with the prediction that the nanocraters are formed by the participation of both the neutralization and the kinetic energy.

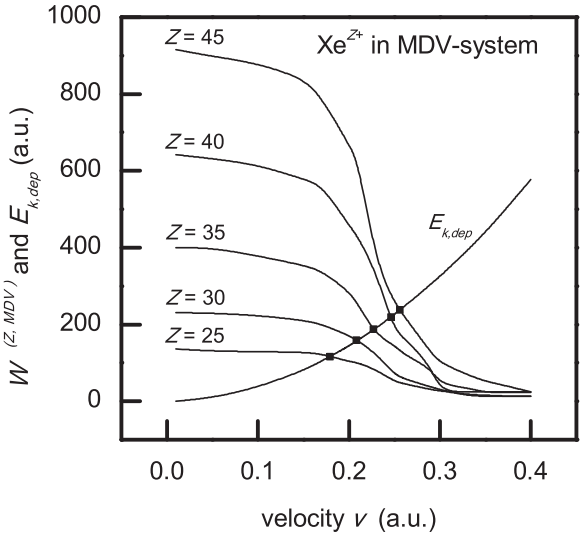

Figure 2: Neutralization energy $W^{(Z,MDV)}$ and deposited kinetic energy $E_{k,dep}$ for Xe^{Z+} ions within the MDV-system (Co + Al_2O_3 film) via ionic velocity v. By symbols we denote the critical velocities v_c for the craters formation.

Acknowledgments

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