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# EFFECT OF THE IONIC TYPE ON THE SHAPE OF THE NANOSTRUCTURES CREATED BY AN IMPACT OF SLOW HIGHLY CHARGED IONS ON GOLD SURFACE

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**Abstract.** We study the interaction of slow highly charged $Ar^{Z+}$, $Kr^{Z+}$ and $Xe^{Z+}$ ions, (charge $Z \gg 1$) with gold surface and propose a theoretical model for determination of the shapes of the obtained surface nanostructures. Within the framework of the model we introduce the critical ionic velocity as a measure of the interplay of the neutralization energy and the deposited kinetic energy, both necessary for the surface nanostructure creation. The influence of the core polarization, i.e. the ionic type on the value of the critical ionic velocity is discussed. The value of the critical velocity we use to define a sufficiently accurate criterion whether the nanohillock or nanocraters are the result of the surface modification, i.e., we predict the shape of the created nanostructure for the particular ionic type.

## 1. INTRODUCTION

Irradiation of solid by swift heavy ions or slow highly charged ions (HCI) results in the nanometric surface modification such as hillock, crater, caldera, pit etc. The condition that has to be satisfied for the production of the particular surface structure is an important information of the surface modification, from the experimental as well as the theoretical point of view. The commonly used theoretical models which describe the surface modification are the molecular dynamics simulations, see Nordlund et al. 2014 and inelastic thermal spike model Toulemonde et al. 1992. Up to now, the theoretical model (energy dissipation model - EDM) confirmed by the experiment that predict the shape of the surface nanostructure has been proposed only for slow highly charged xenon ion impacting upon a gold surface (Majkić et al. 2021). The EDM is based on the quantum two-state vector model and micro staircase model for the neutralization energy calculation and charge dependent ion-atom potential model

for the kinetic energy loss calculation. The model enable us to define the critical velocity for various ion-surface combinations. We analyze the influence of the core polarization on the value of the critical ionic velocity as well as on the shape of the formed surface nanofeatures.

## 2. SHAPE OF THE NANOSTRUCTURE

We consider the highly charged $Ar^{Z+}$, $Kr^{Z+}$ and $Xe^{Z+}$ ions impinging upon a gold

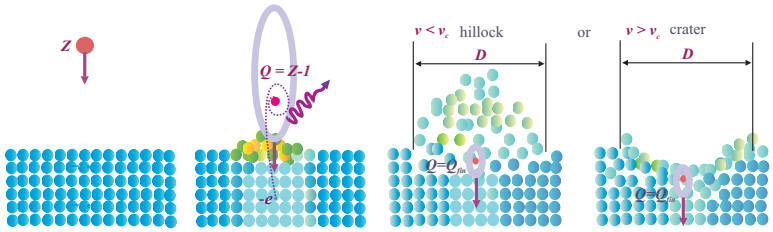


Figure 1: Schematic description of the nanohillock ($v < v_c$) and nanocrater ($v > v_c$) formation during the interaction of HCI with gold surface.

surface at low to moderate ionic velocity. For the same charge $Z$, the considered ions have different electronic core structures. The energy necessary for the surface nanofeatures creation within the EDM consists of the neutralization energy and the deposited kinetic energy, both dependent on the ionic electronic core structure.

Above the surface, the neutralization process is quantified by the population probability for the electron capture from the metal into the highly excited (Rydberg) state; the process we consider as an electron tunnelling through the potential barrier formed between the solid and the ion. We solve the time-dependent Schrödinger equations with in- and out- Hamiltonians $\hat{H}_1$ and $\hat{H}_2$, see Nedeljković et al. 2007. In the treatment of the intermediate stages of the neutralization process the polarization of the electronic cloud of the ionic core is taken into account via the appropriate interaction of the Simons-Bloch type of the active electron and the ionic core. This interaction governed the out Hamiltonian $\hat{H}_2$. Outside the solid, the in Hamiltonian $\hat{H}_1$ describes the electron interaction with polarized solid; inside the solid, the electron is in the mean field described by the potential well of the Somerfield model of the solid. The more accurate treatment is to solve the Schrödinger equation for a particle in the one-dimensional lattice with the periodic potential within the framework of the homotopy perturbation approach, see Kevkić et al. 2019. Within the framework of the micro staircase model (in which the fine structure of the neutralization cascade of the ions approaching the solid surface is taken into account) the initial ionic charge reduces in time: $Q = Z \to Q = Z - 1 \to ... \, Q(R) \to ... \to Q_{fin}$, see Fig. 1. The core polarization modifies the population probabilities and the corresponding neutralization distances, while the final ionic charges $Q_{fin}$ are almost the same, see Majkić et al. 2019. The neutralization energy $W^{(Z,MV)} = W_{Z,pot} - W_{Q_{fin}^{MV},pot}$ defined as difference of the initial and final potential energies, depends on the ionic type via the initial potential energy.

Inside the solid, the deposited kinetic energy into the active interaction volume of depth $\Delta x$ is given by $E_{k,dep} = (dE_n/dx)\Delta x$ (see Majkić et al. 2021). Nuclear

stopping power $dE_n/dx$ we calculate using the charge dependent interaction between the HCI and target atoms. This interaction is significantly different for different ionic types, due to different nuclear charges of the considered ions.

The facts that both the neutralization energy and deposited kinetic energy are sensitive to the ionic type, directly influences on the nanosturcture shape. That is, the critical ionic velocity $v_c$:

$$W^{(Z,MV)}(v_c) = E_{k,dep}(v_c), \tag{1}$$

separates the velocity region into two subregions: for very low ionic velocities ($v < v_c$) the EDM predicts the hillocks as a dominant structures, while for the velocities larger than the critical one ($v > v_c$), expected structures are craters. In the first case (hillock formation), the neutralization energy has a dominant influence in the surface modification, while the main contribution in the surface nanocraters formation is given by the deposited kinetic energy.

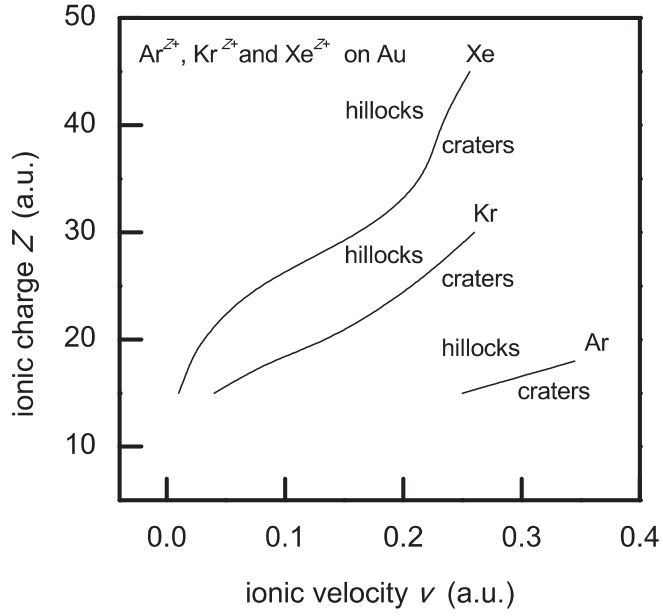


Figure 2: $\{Z-v\}$ diagram for $Ar^{Z+}$, $Kr^{Z+}$ and $Xe^{Z+}$ ions, $Z = 15, 18, 20, 25, 30, 35, 40$ and 45, interacting with gold surface. Solid curves are the kritical velocities.

## 3. RESULTS

The critical velocities enable us to analyze the effect of the ionic type on the shape of the nanofeatures created by the impact of slow HCI on the metal surface.

In Fig.2. we present the $\{Z - v\}$ diagram with critical ionic velocity $v_c$ for $Ar^{Z+}$, $Kr^{Z+}$ and $Xe^{Z+}$ ions impacting upon the Au target. From figure one can see the decreasing character for the critical ionic velocities with increasing of the core polarization ($Ar^{Z+} \rightarrow Kr^{Z+} \rightarrow Xe^{Z+}$) for the same ionic charge $Z$. According to $\{Z - v\}$

diagram, for example, the interaction of the $Kr^{30+}$ ions with gold surface at velocity lower than $v_c = 0.26$ a.u. results in a hillock formation, while $Xe^{30+}$ ions at velocities $v = 0.26$ a.u forms the craters. The $Ar^{18+}$ ions in the interaction with gold target will form craters for velocities larger than $v_c = 0.34$ a.u., while $Kr^{18+}$ and $Xe^{18+}$ ions create the same structure for velocities larger than $v_c = 0.09$ a.u. and $v_c = 0.02$ a.u., respectively.

The predicted types of the nanostructures are in accord with the experimental results for the interaction of the $Xe^{Z+}$ ions with gold targets (Stabrawa et al. 2017, Stabrawa et al. 2022, Pomeroy et al. 2007). The critical velocities for other ion-target combinations can be also obtained from our model. The agreement is also obtained for $Xe^{Z+}$ ions interacting with titanium targets (Stabrawa et al. 2017, Majkić et al. 2021). From the $\{Z - v\}$ diagrams one can tune the velocity needed for the particular surface structure formation by an impact of the ion of a given charge $Z$.

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