Publ. Astron. Obs. Belgrade No. 102 (2022), 125 - 128 *Contributed Paper*

THE INFLUENCE OF THE ION-TARGET PARAMETERS ON THE SIZE OF THE SURFACE NANOHILLOCKS CREATED BY AN IMPACT OF HIGHLY CHARGED IONS

N. N. NEDELJKOVIĆ[1], M. D. MAJKIĆ[2], M. A. MIRKOVIĆ[3], I. STABRAWA[4(a)] and D. BANAŚ[4(b)]

[1] *University of Belgrade, Faculty of Physics, P.O. Box 368, 11001 Belgrade, Serbia*
E–mail hekata@bg.ac.rs

[2] *University of Priština-Kosovska Mitrovica, Faculty of Technical Sciences, Knjaza Miloša 7 38220 Kosovska Mitrovica, Serbia*
E–mail milena.majkic@pr.ac.rs

[3] *Academy of Technical and Art Applied Studies, College of Applied Studies of Civil Engineering and Geodesy, Hajduk Stankova 2, 11050, Belgrade, Serbia*
E–mail marko.a.mirkovic@gmail.com

[4] *Jan Kochanowski University, Institute of Physics, Uniwersytecka 7, 25-406 Kielce, Poland*
E–mail (a)i.stabrawa@ujk.edu.pl
E–mail (b)d.banas@ujk.edu.pl

Abstract. We study the interaction of slow highly charged Xe^{Z+}ions (charge $Z \gg 1$) with gold and titanium targets and propose the theoretical model of the surface nanohillock formation for low to moderate ionic velocities. We apply the quantum two-state vector model accompanied by the micro staircase model for the neutralization energy calculation; the nuclear stopping power we consider using the charge dependent ion-atom interaction potential. We propose the cohesive energy dissipation model for the calculation of the diameter of the considered nanohillocks. The effect of the ionic charge, velocity and target type on the size of the nanostructure is demonstrated.

1. INTRODUCTION

Theoretical and experimental studies of the surface nanostructure creation by an impact of the slow highly charged ions (HCI) have a diverse applications in a surface and material science. Theoretical studies that appears in the literature are mainly based on the molecular dynamics simulations (Nordlund et al. 2014) and the inelastic thermal spike model (Toulemonde et al. 1992). The theory concerning the metal-surface modification has been developed using the energy dissipation model (EDM); the model consists of the quantum two-state vector model accompanied by the micro-staircase model of the HCI neutralization, and the charge dependent model of the kinetic energy loss (Nedeljković et al. 2016, Majkić et al. 2021). The experimental

studies of the nanostructuring of the metal surface have been recently performed, see Stabrawa et al. 2017.

The aim of the present contribution is the calculation of the diameter of the surface nanohillocks that can be compared with experiment. The effect of the ion-target parameters (ionic charge, ionic velocity and the target type) on the size of the nanostructure we analyze within the framework of the EDM.

2. COHESIVE ENERGY DISSIPATION MODEL

We consider the highly charged Xe^{Z+}ions, (charge $Z \gg 1$) impinging upon a metal

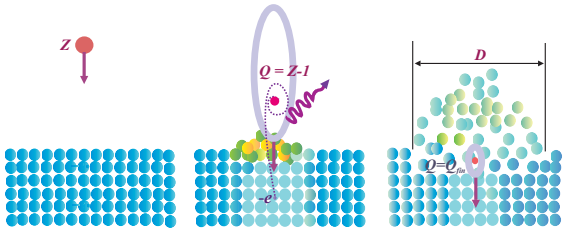

Figure 1: Schematic description of the nanohillock formation during the interaction of HCI with metal surface.

surface at a velocity in the range from very low to moderate. The interaction of the ions with the surface can be divided into two stages. In the first stage, the ions approach the surface and the cascade neutralization of the ions above it occurs, see intermediate stages of the ion neutralization presented in Fig. 1. This process is accompanied by the neutralization energy deposition. Below the surface the process of the elastic collisions of the projectile with target atoms is the main mechanism of the energy dissipation. The kinetic energy of the ions in the form of the kinetic energy loss is deposited into the surface. Both energies contribute to the surface modification. The shape of the nanostructure depends on the interplay of these two energy contribution, described by the critical ionic velocity v_c. The hillock-like structures appears for velocities $v < v_c$, for which the neutralization energy dissipation has a dominant role.

Within the EDM, the total deposited energy $E_{tot,dep}$ into the active volume V of the target consists of the neutralization energy and the deposited kinetic energy $E_{tot,dep} = W^{(Z,MV)} + E_{k,dep}$. Deposited energy during the surface modification is responsible for an increase of the target energy: $E_{tot,dep} = E_{fin} - E_{in}$, where E_{in} and E_{fin} describe the initial and the final state of the target. Within the framework of the cohesive energy dissipation model, the bounds between the target atoms change during the solid modification: $E_{in} = -E_{c0}$ and $E_{fin} = -E_c$, respectively, where E_{c0} and E_c are the absolute values of the cohesive energies of unperturbed (initial) and perturbed solid (final).

Therefore, $E_{tot,dep} = E_{c0} - E_c$, where $E_{c0} = n_0 U_0 V$, where n_0 and U_0 are the initial atomic density and (absolute value) of the corresponding cohesive energy per atom and $E_c = nU(V + V_h)$ where V_h is the hillock volume, n is the final atomic density and U is the (absolute value) of the corresponding cohesive energy per atom. The mass of the initial active volume V is distributed to the volume $V + V_h$, so that

$n_0V = n(V + V_h)$ and $E_c = n_0UV$. The total deposited energy in the considered model is given by $E_{tot,dep} = n_0(U_0 - U)V$ The energy $E_{tot,dep}$ can be expressed as a part of the (absolute value) of the initial cohesive energy E_{c0}:

$$E_{tot,dep} = \kappa_c E_{c0}, \kappa_c = \frac{U_0 - U}{U_0}, \tag{1}$$

where κ_c represents the degree of the surface modification. This parameter κ_c can not be directly obtained from our model (for each Z and v and particular target, one can estimate the parameter κ_c that exactly fits the experiment).

The active volume $V = (D^2/4)\pi\Delta x$ in which the energy is deposited we consider as a cylinder of diameter D with the high equal to the interaction depth Δx. For gold and titanium targets $\Delta x \approx 5\bar{c} \approx 38.5$ a.u. and $\Delta x \approx 5\bar{c} \approx 33.2$ a.u., respectively (see Majkić et al. 2021), where c is the mean lattice constant. In the first approximation diameter D coincides with the diameter of the formed nanohillock. According to the relation (1) for the nanohillock diameter we get a simple expression

$$D = 2\sqrt{\frac{E_{tot,dep}}{\pi\epsilon_{c0}\kappa_c\Delta x}}, \tag{2}$$

where $\epsilon_{c0} = n_0U_0$ is the (absolute value) of the initial cohesive energy density.

The cohesive energy per atom and the atomic density of the unperturbed gold and titanium are $U_0 = 3.93$ eV$= 0.144$ a.u., $n_0 = 8.7 \cdot 10^{-3}$ a.u., and $U_0 = 4.85$ eV$= 0.1783$ a.u., $n_0 = 8.4 \cdot 10^{-3}$ a.u., respectively.

3. RESULTS

We analyze the size of the nanohillocks created on the titanium and the gold nanolayers by an impact of slow Xe^{Z+} ions, $Z = 20, 25, 30, 35, 40$ and 45. The nanolayers are strongly perturbed during the ionic motion and the process of the nanostructure formation, what is described by the degree of the target modification κ_c. The values fitting the available experiments (see Stabrawa et al. 2017) are $\kappa_c = 0.05$ for titanium and $\kappa_c = 0.043$ for gold targets.

In Fig. 2 we present the nanohillock diameters calculating according to (2) for Ti and Au targets. From Fig. 2 we can recognize the decreasing behaviour of the nanohillock diameter D with increasing of the ionic velocities v, similar to the behaviour of the neutralization energy. This can be explained by the dominant influence of the neutralization energy on the creation of the nanohillocks for low ionic velocities $v < v_c$. Also, for both types of targets, the nanohillock diameters increase with increasing the ionic charge. According to the relation (2) the type of the target has the significant influence on the nanostructure size. For the same Z, hillock diameters obtained on Au target are systematically larger than those obtained on Ti surfaces. Namely, the energy density $\epsilon_c = \kappa_c\epsilon_{c0}$ of the gold target $\epsilon_c = 5.4 \cdot 10^{-5}$ a.u. is smaller than the energy density of titanium $\epsilon_c = 7.5 \cdot 10^{-5}$ a.u, so that, according to the relation (2) the nanohillock diameter is larger.

Acknowledgments

This work was supported in part by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project 171016, 171029). D. Banaś

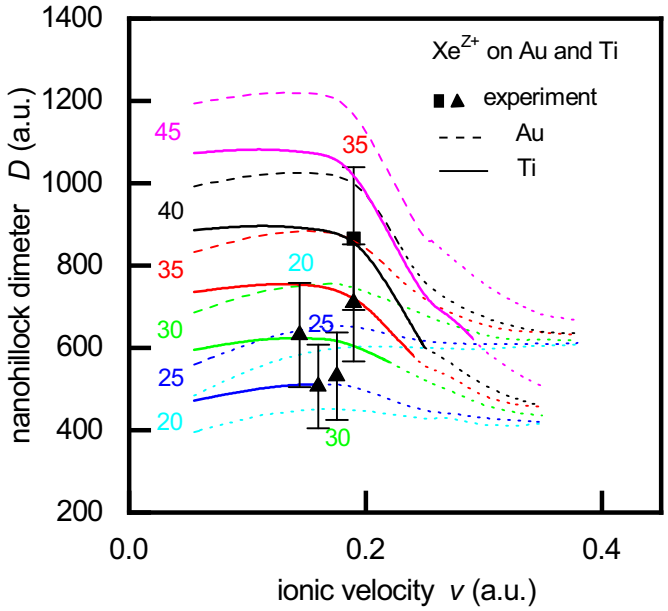

Figure 2: Diameter of the nanohillocks formed on the titanium and the gold targets by an impact of the Xe^{Z+} ions, $Z = [20, 45]$, versus ionic velocity. Solid and dashed curves are for $v < v_c$ and Ti ($\kappa_c = 0.05$) and Au ($\kappa_c = 0.043$) targets, respectively, and dotted curves are for $v > v_c$. Full triangles (Ti) and square (Au) are the experimental values, see Stabrawa et al. 2017.

and I. Stabrawa are grateful for the financial support of the European Regional Development Fund in the framework of the Polish Innovative Economy Operational Program (contract no. WNP-POIG.02.02.00-26-023/08) and the Development of Eastern Poland Program (contract no. POPW.01.01.00-26-013/09-04) for the purchase of the equipment.

References

Majkić, M. D., Nedeljković, N. N. : 2021, *Vacuum*, **190**, 110301. Nedeljković

Nedeljković, N. N, Majkić, M. D., Božanić, D. K., Dojčilović, R. J.: 2016, *J. Phys. B: At. Mol. Opt. Phys.*, **9**, 125201.

Nordlund, K., Djurabekova, F.:2014, *J. Comput. Electron.*, **13**, 122141.

Stabrawa, I., Banaś, D., Kubala-Kukuś, A., Szary, K., Braziewicz, J., Czub, J., Jabłoński, Ł., Jagodziński, P., Sobota, D., Pajek, M., Skrzypiec, K., Mendyk, E., Teodorczyk, M.: 2017, *Nucl. Instrum. Methods Phys. Res. B* , **408**, 235-240

Toulemonde, M., Dufour, C., Paumier, E.: 1992, *Phys. Rev. B*, **46**, 14362.