Theoretical model for the nanohillocks and nanocraters formation on the metal surface by an impact of slow highly charged ions

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Nanohillocks and nanocraters, created as a response of the metal surface on the highly charged ions irradiation, are theoretically studied using the cohesive energy model (CEM). In the first step of the CEM we consider a deposition of the neutralization and the kinetic energy into the solid. We employ the quantum two-state vector model (TVM) [1] of the intermediate Rydberg state population and the micro-staircase model [2] of the cascade neutralization above the surface, and the charge dependent ion-atom interaction potential model for the calculation of the kinetic energy loss as a result of the elastic collisions between the projectile and the target atoms below the surface [2]. The synergy of the neutralization energy and the deposited kinetic energy in the process of the nanostructures formation is described by the critical ionic velocity [2]. For ionic velocities lower than the critical one, model assumes an appearance of the hillocks, and the neutralization energy gives the main contribution in the surface modification, while for the larger velocities the deposited kinetic energy plays a dominant role and the expected structures are craters [3].

In the second step of the CEM, we assume that the total energy (consisting of the neutralization energy and the deposited kinetic energy) deposits into the active volume of the solid, resulting in a decrease in the target cohesive energy. In the case of hillock formation (expanded metal), the modified interatomic distances and the change of the electron density profile affect the decrease of the bonding strength. The rearrangement of atoms leads to the rise of the volume above the surface and hillock creation. The process below the surface has a negligible contribution. On the other hand, for crater formation the atomic collisions below the surface play a dominant role. In the final state of the surface modification, the bond strength between target atoms inside the crater volume tends to zero and a number of atoms are ejected from the surface, while the remaining part of the active volume is totally recovered. The proposed simple mechanism enables us to calculate the nanostructure diameters. The results are consistent with the experiments related to the hillock [4] and crater [3] nanostructures, formed on the titanium and gold targets.

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