The Simulation of Ion Bombardment on the Ti$_{13}$ Clusters with Pair Interatomic Interaction$^1$

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Abstract – The method of molecular dynamics was used for simulating ion bombardment on the titanium nanoclusters with pair interatomic interaction (Morse potential). The energy of the bombarding particles varied from 100 to 1000 eV. The ion-cluster interaction was studied for various impact parameters. The ion energy distribution function and ion escape direction function have been established.

1. Introduction

When modifying the rigid body surface by arc discharge low-temperature plasmas in the surface there occurs the clusters of metals MeN (N – number of atoms in a nanocluster). The clusters comprise the elements of the cathode and substrate materials [1–3]. Moving in an ion-plasma flux the clusters suffer from elastic and not elastic encounters with various high-energy particles (atoms, ions, molecules, etc.). The resulting changes of the value and direction of interacting particles speeds cause shifts of the spatial and time characteristics of the low-temperature plasmas.

The goal of the work is the molecular-dynamic simulation of the initial interaction stages of the titanium ions (atoms) with nanoclusters Ti$_{13}$. By the term of the period of the oscillations of atoms for a wide range of temperatures. Thereof, when computer stimulating we did not consider the cluster atoms thermal motion its temperature was considered equal to zero. Thermostatting of the prototype system was not used. Non elastic losses of the ion energy while interacting with the cluster atoms were not considered. The angel $\Theta$ was counted off from the direction of the ion initial motion.

2. Model

The initial clusters configuration was chosen as casual distribution of the titanium atoms in space. Then, the structure was relaxed by the minimization of the total potential energy by Metropolis method at the predetermined temperature [6]. The interactions between the nanocluster atoms and the ion with the cluster were described by means of Morse pair potential [7]:

$$V(r) = D\{\exp[-2\alpha(r - r_0)] - 2 \exp[-\alpha(r - r_0)]\},$$

which parameters $\alpha$, $r_0$, and $D$ for the titanium are equal to 1.05291 Å$^{-1}$, 3.230 Å, and 0.49888 eV, respectively [8].

To solve the system of the equations for the particles motion there was used Verlet algorithm in “the high-speed form” [9] with a variable time step. To implement this method the values of speed $v_i^{\text{old}}$ and coordinates $r_i^{\text{old}}$ at $i + 1$ time step for $k$ cluster atom or the ion are calculated as:

$$r_i^{\text{new}} = r_i^{\text{old}} + v_i^{\text{old}}\Delta t + \frac{F_i^{(k)} + F_i^{(l)}}{2m_i^{(k)}}\Delta \tau^2,$$

$$v_i^{\text{new}} = v_i^{\text{old}} + \frac{F_i^{(k)} + F_i^{(l)}}{2m_i^{(k)}}\Delta \tau,$$

where $v_i^{(k)}$, $r_i^{(k)}$ are the values of the speed and the coordinates of the particle for $i$-step; $m_i^{(k)}$ is the weight of $k$ atom (ion); $\Delta \tau$ is the time step; $F_i^{(k)}$, $F_i^{(l)}$ are the values of the forces acting on $k$ atom (ion) at $i$ and $(i + 1)$ time step, respectively. The time step was chosen so that the motion for the time interval under dealing with did not exceed 5% of the minimal distance in the ion-cluster system.

All the design values were averaged after examining 10000 ion-cluster interactions for various initial

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titanium nanocluster configurations. When interacting the nanocluster rotated around the coordinate axes by the angels drawn at random. The ion joined in the cluster if the ion’s kinetic energy was less than the potential energy of the bond (negative) with the cluster atoms, and if it did not leave the cluster atoms for 10000 time steps. The ion was reflected from the cluster or past through it if the distance up to the nearest cluster atom was more than 10 Å, and if the speed was directed from the center of the cluster mass.

3. Discussion of results

1. The central impact \((b/R = 0)\). The analysis of various cluster configurations (in Fig. 1 the example of a configuration is presented) shows that in early the ion interacts with the nearest to it and central cluster atoms, which are imparted the maximal kinetic energy. The further energy redistribution inside the cluster occurs due to the subsequent development of the cascade of collisions. The dependence of the cluster-ion system energies on the time of interaction is shown in Fig. 2 for the configuration of atoms (Fig. 1) (initial energy of the atoms 100 eV). The final energy redistribution between nanocluster atoms is shown in Fig. 3. As noted increasing ion energy is accompanied by increasing the quantity of the passed/reflected particles and decreasing the time of their interaction with the cluster atoms. Upon that there is the increase of the average energy of the reflected ions from \(0.41 E/E_0\) for 100 eV to 0.98 \(E/E_0\) for 1 keV \((E_0\) is the initial energy of the ions, \(E\) is the final energy of the ions).

In Figs. 4 and 5 there are the functions of escape directional distribution of the ions \(f(\Theta)\) and of the energy distribution \(f(E)\) after the ion–cluster interaction for various initial speeds. It is possible to divide the particiles energy distribution \(f(E)\) into three bands of energy: 1) from 0 to 0.05 \(E/E_0\); 2) from 0.05 to 0.30 \(E/E_0\); 3) from 0.30 \(E/E_0\) and above. The division is caused by various contributions to the resultant energy distribution of the particiles condensed on the cluster, reflected and past through nanocluster ions. In addition each energetic band is characterized by the pronounced maxima.

For the first energy band the equal distribution of ion escape directions from the cluster is observed. In addition this band is described by the sum of all mentioned above particles. The position of the maximum in this band has no strict correlation with the ion energy. The second band is characterized by the reflection of the ions from the cluster by the angels more then 120º with respect to the initial direction of the titanium atom movement. The occurrence of the energy maximum in this band is caused by the interaction of the ion with the central cluster atom (12th atom in Fig. 1). The increase of the ion initial speed is accompanied by its displacement in high-energy region \(E/E_0\) (from 0.15 for 100 eV to 0.23 for 500 eV). When the energy of the bombarding ions is more than 500 eV the ion does not escape. The third band \(f(E)\)
causes the occurrence of the angular distribution maximum for the angels $\Theta$ in the interval 10 to 50º and about 100º. The maximum in the third band is caused the fact of the ion scattering by the angels about 41º while the ion position shifts from 0.54 (175 eV) to 0.99 $E/E_0$ (1 keV). Besides in the process of the energy increasing the angular distribution $f(\Theta)$ typical for the third energy maximum displaces in the smaller angle region, i.e the quantity of the ions past through the cluster increases. The contribution of the ions with the angel of reflection about 100º gradually decreases, and if the energy is above 300 eV there are not such ions. The second and third bands are characterized only by the atoms reflected from the cluster surface or by past through it ones. Under increasing the initial ion speed the quantity of the ions with the energies typical for the first (from 17% for 100 eV to 1% for 500 eV) and he second (from 48% at 100 eV to 3% at 500 eV) energy bands decrease.

2. Noncentral collision ($b/R \neq 0$). In Fig. 6 the dependence of the ion passing $\alpha$ on the relative impact parameter $b/R$ is shown. The behavior ($b/R$) may be explained by the cluster structure features (Fig. 1). In the cluster under examining three layers (from the central plane) divided by two intervals may be described. After striking into the specified intervals the ion penetrates deeper into the cluster and passing through it loses more energy, and therefore the probability to join in the cluster increases together with the decrease of the passing factor. When the ion strikes in a layer it transfers its kinetic energy to the nearest atom, and the ion, as a rule, is reflected or for greater initial speeds passes through the cluster.

The increase of the relative impact parameter $b/R$ is accompanied by the increase of the maximum intensity in the third energy band (Fig. 7) and its gradual displacement to the great value region $E/E_0$ is observed. In addition the decrease of this maximum width is observed. For small initial ion energies the dependence of the third zone maximum intensity on the values $b/R$ correlates with the behavior of the factor ion passing through the cluster. Thus the quantity of the back scattered ions (> 90º) decreases and for $b/R > 0.3$ there are not the ions with angel of reflection of more than 120. In the ion energy distribution the second energy band maximum disappears even when there is insignificant deviations from the central impact ($b/R \geq 0.1$).
4. Conclusion
The results of the computer stimulation of the titanium ion–nanocluster interaction make it possible to draw the following deductions:

1. Initially the ion interacts with the central and the nearest to the central nanocluster atoms. The further energy redistribution between the cluster atoms is caused by the development of the cascade of collisions. The increase of the initial energy of the particles bombarding on the cluster leads to the increase of the ion passing factor, the quantity and relative energy of the reflected ions. Upon that the decrease of the interaction time is observed.

2. After the ion-cluster interaction the energy distribution of ions may be divided into three energy bands: 1) from 0 to 0.05 $E/E_0$; 2) from 0.05 to $E/E_0$; 3) from 0.30 $E/E_0$ and above. The division is caused by various contributions to the resultant energy and angular distribution of the particles condensed on the cluster, reflected and past through it atomic particles. The increase of the falling ion energy leads to the decrease of the first and second energy bands contributions to the resultant energy spectrum. In all considered energy bands after ion-cluster interactions there are the maxima conforming to various angels of the ion distribution.

3. The dependence of the passing factor on the impact parameters is caused by the structural features of the nanocluster. The increase of the impact parameters causes the increase of the maximum intensity in the third energy band and the decrease of the maxima in the first and second energy bands.

References