SURFACE NANORELIEF MODIFICATION OF CONSTRUCTIONAL MATERIALS AT LOW ENERGY ION BOMBARDMENT

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Process of thermal smoothing at bombardment of metal surfaces by low energy heavy ions is investigated. It is shown, that smoothing can occur in nonlocal thermoelastic peak of ion under action of forces of surface tension at spreading the melted material on the surface. The model of thermal smoothing alternative to model of ion polishing due to ion sputtering of target atoms is developed. Criteria of applicability of model for any combination "ion–target", and analytical expressions for basic parameters of process of smoothing (size of smoothing area created by single ion, time of smoothing) are received.

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INTRODUCTION

Interest to physical processes on the surface of materials at ion bombardment is associated with the development of nanotechnologies, requiring tools for its realization, ability to create and/or modify the nano-sized objects. Especially it is important for fine finishing of sample surfaces and manufacturing of details in the size less than 100 nanometers [1].

It is known that ion bombardment can lead to smoothing of surface relief of solid target. Smoothing processes were associated with ion sputtering and considered in the approximation of linear theory of collision cascades valid only at low density of binary collisions [2]. So, the relief smoothing was explained by preferential sputtering of hillocks and smoothing of hollows due to accumulation there atoms sputtered from the surface of adjacent areas, as well as the atoms ejected from their places by the ion bombardment and diffusing on the surface [3].

However, at sufficiently high density of collisions in cascades the process of modification of metal surface can get qualitatively different character obeying the laws of thermodynamics and continuum mechanics. Smoothing processes as well as surface roughening processes of the amorphous metal target bombarded by heavy ions at MeV energies were considered in [4]. It was shown that the change in the morphology of the irradiated surface is mainly due to collective effects of formation of ion thermal peaks, as the result of viscous flow of target material in the thermal peaks. It is interesting to consider from similar viewpoint processes of surface smoothing of metal target under the action of heavy ions of low energy E ~ 1...30 keV.

Interaction of heavy low-energy ion with solid body leads to formation around ion trajectory superheated nanometer-sized region – nonlocal thermal peak (NTP) [5]. The energy density ε in NTP depends on species and energy of the ion as well as on parameters of target material. As show estimations, ε can exceed the value necessary for target material melting. In this case smoothing of curved surface which adjoins to NTP can occur due to material flow under the action of surface tension. It is supposed that there is no ejection of molten material from peak volume and formation of damages on target surface.

The purpose of this work is determination of physical conditions and basic parameters of smoothing process of metal surface by heavy ions of low energy in the model of nonlocal thermal peak of the ion, and analysis of the possibilities of its practical use for smoothing nanometer-sized irregularities on the surface of construction materials with different structures.

NANORELIEF SMOOTHING IN MODEL OF NONLOCAL THERMAL PEAK OF ION

The simulation results using SRIM2008 program package showed that singly connected subsurface cascade of excited atoms with stored phonon energy $E_{ph}(E)=\eta(E)E$ is formed at low-energy heavy ion incident on the target surface. Here $\eta(E)$ is relative part of phonon loss of ion energy *E*. The peak arising on the basis of such a cascade can be approximated by a spherical segment with the center in the middle of the average length of ion projected range *l*(E) and with initial radius $R(E,d)=l(E)/2+R_T(d)$ where R_T is the radius of thermal spreading of point heat source. R_T is determined by the diffusion of thermal phonons during the ion-ion relaxation time τ, and depends on the effective size of target crystallite *d*. Temperature and phase state of the material in volume *V* of spherical NTP are determined the average density of thermal energy $\varepsilon\left(E,d\right)= E_{ph}(E)/V\left(E,d\right)$.

Such approach for the description of physical processes arising at ion interaction with solid body, remains valid in following range of energies:

$$E_{\min} \le E \le E_{NTP}. \qquad (1)$$

The maximum permissible energy E_{NTP} characterizes the qualitative change in cascade structure, leading to the formation of several weakly connected overheated areas. The minimum energy $E_{\min}$ is determined by the opportunity of the thermodynamic description of the physical processes in the NTP [5].

Smoothing the target surface in the ion NTP is possible with obligatory fulfillment of several conditions. First of all, the initial density of thermal energy ε at the peak should exceed energy density $\varepsilon_{m2} = \rho C\left(T_m-T_0\right)+\rho q_m$ required to melt the material in the NTP volume. Here T_0 is initial temperature, T_m is melting point of the target material, ρ, C and q_m are the mass density, the specific heat and the specific heat of melting of target material, accordingly. In the sequel, NTP "spreads thermally" increasing its radius and decreasing density of thermal energy and average temperature.

Secondly, the effective smoothing is possible only under the condition that the lifetime of molten region τ_T exceeds the time τ_D necessary for smoothing of the curved surface by surface tension forces. Estimates indicate that the condition is usually satisfied for nanometer-sized thermal peaks in metals.

Finally, it is necessary to ensure the conditions excluding the droplet sputtering and cratering. Ejection of melted material with cratering is impossible if elastic energy W_{el} spent on drop ejection does not exceed the energy W_s spent on formation of droplet and crater surfaces [5]. In addition, it is necessary to satisfy the condition $\varepsilon < \varepsilon_{b1}$, where ε_{b1} is the energy density of the start boiling, as the boiling also leads to the vaporization and cratering of target surface.

Thus, smoothing effect of the NTP takes place in energy ranges determined by relation (1), and also at satisfying the following conditions:

$$\varepsilon_{m2} \le \varepsilon\left(E,d\right) \le \varepsilon_{b1} \quad , \tag{2}$$

$$W_{el}\left(E,d\right) < W_s\left(E,d\right). \tag{3}$$

In order to estimate the parameters of the smoothing process (Fig. 1) we also suppose that thermal peak maintains sphericity and position of center during thermal spreading. Maximum radius R_s of the molten region which determines the smoothing effect of the thermal peak, calculates from the equation $\varepsilon(E,d) = \varepsilon_{m2}$:

$$R_s\left(E\right) = k_s \sqrt[3]{\frac{3\eta\left(E\right)E}{4\pi\rho\left[C\left(T_m - T_0\right) + q_m\right]}}\,, \tag{4}$$

where k_s is the coefficient taking into account the shape of the forming peak. The value k_s weakly varies (between 1.0 up to $\sqrt[3]{2}$) at the change of peak shape from spherical to hemisphere. In following calculations we assume k_s =1.1. Diameter of thermally smoothing area of single ion (see Fig. 1) is equal to $D_s\ E\ = \sqrt{4R_s^2 - l^2}$.

Let's estimate the smoothed volume by example of smoothing of hemispherical hillock in radius R_a (see Fig. 1). The smoothed volume V_1 has the shape of spherical segment in height h_s and radius R_a and in this approximation is equal $V_1 = \pi h_s{}^2 R_a$. At $R_s << R_a$, average height h_s smoothed by thermal peak of single ion on spherical irregularity, may be taken as:

$$h_s\left(E\right) \approx \frac{R_s^2\left(E\right)h_{min}}{R_a{}^2}\left(1 - \frac{l^2}{4R_s{}^2}\right)^2 ln\frac{R_a}{2h_{min}}\,, \tag{5}$$

where $h_{\min}$ is the final height of roughness, at which the smoothing process is terminated.

Fig. 1 displays scheme of formation of subsurface melted region of radius R_s at incidence of single low-energy ion on convex surface of hillock of radius R_a.

The smoothing time t_s of the target surface can be estimated on the basis of the volume $V_a \approx \pi R_a / 6$ of the roughness of target surface and the rate of volume smoothing $V_s = jV_1$:

$$t_s\left(E\right) = \frac{V_a}{V_s} = \frac{1}{6\,jh_s{}^2}\,. \tag{6}$$

Here j is the density of ion flow falling normally on target surface.

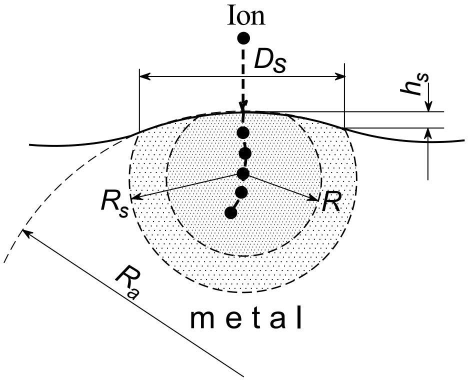


Fig. 1. Scheme of formation of subsurface melted region at incidence of single ion on hemispherical hillock

RESULTS AND DISCUSSION

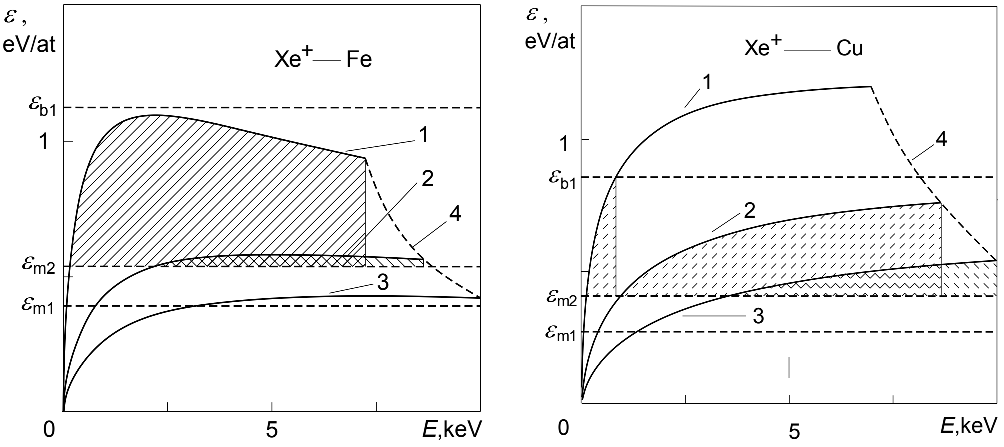
The simulation performed using the program package SRIM2008 has permitted to determine the shape and geometry parameters of the NTP generated in targets of constructional materials (Al, Fe, Zr, Cu, Ag, Au) at normal incidence of ions Ar $^{+}$(Xe^{+}) with energy $E \le E_{NTP}$ on the target surface, the phonon loss of ions E_{ph} and the maximum permissible energy E_{NTP} for various targets.

These parameters permitted to determine all other ones necessary for analysis of smoothing ability of the ion bombardment.

Fig. 2 shows dependences of the energy density ε in the NTPs of Xe^{+} ions on their energy E for the amorphous, nanocrystalline (d = 2 nm) and polycrystalline targets of Fe (see Fig. 2,a) and Cu (see Fig. 2,b) (curves 1–3 respectively). The hatching marks energy ranges where thermal smoothing is possible. The dotted line 4 limits the applicability of the NTP model from high energies and corresponds to the maximum permissible *E*.

As one can see from Fig. 2,a, condition (2) for polycrystalline iron target is not satisfied. Thermal smoothing effect can be observed for copper targets with different structures (see Fig. 2,b). The minimum threshold energy E_1 of thermal smoothing increases with crystallite size *d*. The maximum threshold energy E_{NTP} also increases with *d*.

Analysis of expressions (4–6) shows that diameter D_s of thermally smoothing area increases and smoothing time decreases with ion energy *E*. Both parameters are weakly dependent on the structure of the target (i. e., on *d*).



a *b*

Fig. 2. Dependence of energy density ε in NTP of Xe^+ ions from energy E for targets of Fe (a) and Cu (b) with various structures

The results allow to estimate diameter D_s of thermally smoothing area formed by single ion, and smoothing duration t_s. So, diameters D_s, corresponding to bombardment of polycrystalline targets of Au and Cu by Xe^+ ions with energies E_{NTP} are equal to 10 and 7 nm, respectively; the average heights h_s of smoothing are 0.03 and 0.015 nm respectively. The time t_s of thermal smoothing of polycrystalline target of Au with the height of roughness R_a = 100 nm and with the final height of roughness h_{min} = 10 nm at the bombardment by Xe^+ ions with flux density j = 1 mA/cm^2 and energy E = 3 keV is equal to $t_s \sim 30$ s. This time is comparable with estimate of smoothing time, resulting in model of atom sputtering [6].

The results of investigations allowing to compare opportunities of thermal smoothing some amorphous (am.) and polycrystalline (cr.) constructional materials by ions Ar^+ and Xe^+, are presented in Table. The sign "+"/"-" indicates that the thermal smoothing is possible/impossible, value ΔE_S defines the range of ion energies (in keV), where thermal smoothing is possible.

Ion ΔE_S, keV	Target					
	Al		Fe		Zr	
	am.	cr.	am.	cr.	am.	cr.
Ar	+ 0.08…0.3	-	+ 0.07…0.43; 1.16…2	-	+ 0.18…4	-
Xe	-	-	+ 0.18…7.5	-	+ 0.11…11	-

Ion ΔE_S. keV	Target					
	Cu		Ag		Au	
	am.	cr.	am.	cr.	am.	cr.
Ar	+ 0.04…0.13	-	+ 0.12…0.32	-	+ 0.06…0.27	-
Xe	+ 0.1…0.6	+ 4.35…10	+ 0.1…0.3	+ 2…~20	+ 0.06…0.75	+ 2.4…~ 30

As seen from Table, the effect of surface thermal smoothing of constructional materials depends on the target structure, physical properties of the target material, and ion species. In the case of crystalline targets criterion of thermal smoothing is satisfied only for heavy materials (Cu, Ag, Au) and ions (Xe^+). For amorphous targets criterion of thermal smoothing is satisfied for all examined combinations of "ion-material" except for the combination "Xe^+ – Al". In case of nanocrystalline targets there is range crystallite size d depending both on material and on ion species, wherein the criterion (2) is satisfied, except combinations "Xe^+ – Al".

CONCLUSIONS

1. Model of thermal smoothing of metal surface at bombardment by heavy low-energy ions alternative to model of ion polishing due to ion sputtering is offered.
2. Criteria are obtained allowing for any combination "ion–target" to determine the ion energy range where the proposed model is applied and thermal smoothing is possible.
3. The analytical expressions for the basic parameters of smoothing process (diameter of thermally smoothing area formed by single ion, the time of smoothing) are obtained.

4. It is shown that the effect of surface smoothing in ion thermal peak depends on structure and physical properties of the target material, species and energy of ion, and can make a significant contribution to the overall smoothing process of metal surface.

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ИЗМЕНЕНИЕ НАНОРЕЛЬЕФА ПОВЕРХНОСТИ КОНСТРУКЦИОННЫХ МАТЕРИАЛОВ ПРИ БОМБАРДИРОВКЕ ИОНАМИ НИЗКИХ ЭНЕРГИЙ

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Теоретически исследовался процесс теплового сглаживания при бомбардировке поверхности металлов тяжелыми ионами низкой энергии. Показано, что выравнивание поверхности может происходить под действием сил поверхностного натяжения при растекании вдоль поверхности расплавленного материала, образующегося в нелокальном тепловом пике. Разработана модель теплового сглаживания, альтернативная модели ионной полировки, за счет ионного распыления. Получены критерии, определяющие применимость модели для произвольной комбинации «ион–мишень», а также аналитические выражения для основных параметров процесса сглаживания (размер области сглаживания, создаваемой одиночным ионом, время сглаживания).

ЗМІНА НАНОРЕЛЬЄФУ ПОВЕРХНІ КОНСТРУКЦІЙНИХ МАТЕРІАЛІВ ПРИ БОМБАРДУВАННІ ІОНАМИ НИЗЬКИХ ЕНЕРГІЙ

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Теоретично досліджувався процес теплового згладжування при бомбардуванні металевих поверхонь важкими іонами низьких енергій. Показано, що вирівнювання поверхні може відбуватися під дією сил поверхневого натягу при розтіканні уздовж поверхні розплавленого матеріалу, що утворюється в нелокальному тепловому піку іона. Розроблено модель теплового згладжування, яка альтернативна моделі іонного полірування за рахунок розпилення іонів мішені. Отримано критерії, що визначають застосовність моделі для довільної комбінації «іон–мішень», і аналітичні вирази для основних параметрів процесу згладжування (розмір області згладжування, яка створювана одиночним іоном, час згладжування).