Study of temperature fields under impact of fine-focused heavy ion beam onto metal substrates structure

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Abstract. Results of the study of temperature fields in micro - and nanoscale structures on metal substrates when exposed to a fine-focused beam of medium-energy heavy ions are presented.

1. Introduction
A problem of creating precision mechanics devices in modern instrument engineering is the search for a high-performance manufacturing technology of formation of regular micro- or nanoreliefs in rolling friction and sliding friction pairs significantly improving their operational characteristics. The analysis of existing technologies shows that one of the most promising methods for forming regular micro- and nanoreliefs is surface treatment with a fine-focused beam of heavy ions. The method has exceptional ecological cleanliness, reproducibility and controllability of treatment parameters.

The dependence of a material structure and ion sputtering rate on temperature during formation of micro- and nanoscale objects on a metal substrate by a focused beam of heavy ions causes the necessity to study temperature fields in the ion beam impact zone and requires research of the physics of the processes occurring. Again, this makes it possible to optimize the operating conditions of ion-beam machines and to provide monitoring of operational parameters on a real time basis.

2. Physical effects in solids when exposed to an ion beam
In the basis of the physical phenomena in solids due to exposure to an ion beam, there are the scattering processes of energy deposited by the beam within the surface layer of matter. The thickness of the layer is small and approximately equals the range of charged particles in a solid. When the substrate is exposed to medium energy ions (50-80 keV), the main energy dissipation channel is the thermal conductivity. Small perturbations of pressure and density then arising propagate much faster than temperature, which allows us to consider the process of heat propagation at constant pressure. The thermophysical characteristics of the environment under such conditions can be considered independent of temperature [1].

Let us consider a temperature increase in the metal substrate on exposure to a finely focused...
beam of heavy ions onto its surface. For calculations we use the classical theory of thermal conductivity, since the ion beam exposure time $t$ is much longer than the thermal stress relaxation time $\tau_0$ (for metals $\tau_0 \sim 10^{-12}$ s). Let us also accept the following assumptions:

1. Thermophysical characteristics of the target (in particular, titanium and molybdenum) do not depend on temperature, since for the metals we are considering as a substrate, changes in the thermophysical characteristics are very small over a wide temperature range.

2. Since the sputtered atom energy is 5-10 eV [2, 7] and the ion beam energy discharge directly to the sputtering does not exceed 5%, then in this case the energy losses of the target sputtered atoms can be neglected.

3. The heat flux by radiation from the substrate surface during the heavy ion beam impact can be ignored.

4. Let us consider the impact of an ion beam on the target as surface heat source $q$, since the range of heavy ions at energies up to 50 keV is tens of nanometers, which is much less than penetration depth of temperature field $\Delta T \approx \sqrt{\alpha \tau}$ ($\alpha$ - the temperature conductivity coefficient, $\tau$ is the beam impact time) for the ion beam exposure time under study.

5. Taking into account that the penetration depth of temperature field $\Delta T$ is smaller than the dimensions of the substrate, we can consider the target as a semi-infinite solid.

3. The calculation of temperature fields on exposure to a fine-focused beam onto a metal substrate

In view of these assumptions, the problem of calculating the temperature fields on exposure of a fine-focused beam can be represented as:

$$c_p \rho \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( Kr \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( K \frac{\partial T}{\partial z} \right)$$

$$T|_{t=0} = T_0$$

$$-K \frac{\partial T}{\partial z}|_{z=0} = q(r), r \leq r_p ,$$

$$\frac{\partial T}{\partial z}|_{z=0} = 0, r \leq r_p ,$$

where $c_p$ is the specific heat capacity, $\rho$ is the density, $K$ is the thermal conductivity coefficient of the target; $r_p$ is the beam radius.

Heat flux $q(r)$ due to the impact of an ion beam on the surface of a solid will be written as:

$$q(r) = j(r)E ,$$

where $j(r)$ is the ion beam current density, $E$ is the beam energy in eV.

For equilibrium distribution of current density $j(r)$, the problem comes down to a heat input through a circle of radius $r_p$. The analytical solution of this problem (1) is:

$$\Delta T(r, z, \tau) = \frac{r_p q}{2K} \int_0^\infty \left( J_0(\lambda r)J_1(\lambda a) \right) \left( e^{-\lambda z} erf_c \left( \frac{z}{2\sqrt{\alpha \tau}} - \lambda \sqrt{\alpha \tau} \right) - e^{\lambda z} erf_c \left( \frac{z}{2\sqrt{\alpha \tau}} + \lambda \sqrt{\alpha \tau} \right) \right) d\lambda ,$$

where $\Delta T$ is the temperature increase over the initial temperature.

On the axial line in [2, 7], a solution is given in the form:
\[ \Delta T(0, z, \tau) = \frac{2 \cdot q \cdot \sqrt{a \tau}}{K} \left[ \text{erf}\left(\frac{z}{2 \sqrt{a \tau}}\right) - \text{erf}\left(\frac{\sqrt{z^2 + r_p^2}}{2 \sqrt{a \tau}}\right) \right] \] (2)

Using the series expansion of function \( \text{erf}\left(\frac{x}{\sqrt{a \tau}}\right) \) at small values of the argument \( \frac{x}{\sqrt{a \tau}} \), one obtains a simplified expression for calculating the excess temperature along the axial line:

\[ \Delta T(0, z, \tau) = \frac{q}{K} \left( \frac{\sqrt{z^2 + r_p^2}}{\sqrt{a \tau}} - z \right) \] (3)

The maximum temperature is attained at the point \( (0,0,\tau) \):

\[ \Delta T(0,0,\tau) = \frac{q r_p}{K} \]

The calculation data from shrewd formula (2) show good agreement with the calculation data from formula (3).

For normal distribution of current density \( j(r) \) described by the function:

\[ j(r) = j_0 \exp\left(\frac{-r^2}{r_p^2}\right), \]

following [5], the solution for the axial line can be written as:

\[ T(0, z, \tau) = \frac{q_{\text{max}} \cdot r_p^2}{K} \sqrt{\frac{a \tau}{\pi}} \int_0^{\infty} \frac{dt}{\sqrt{4at + r_p^2}} e^{-\frac{z^2}{4at}}, \]

where \( q_{\text{max}} = j_0 \cdot E \).

Accordingly, for the point with maximum temperature \( (0,0,\tau) \) in the case of normal distribution, the excess temperature will be determined as:

\[ \Delta T(0,0,\tau) = \frac{q_{\text{max}} \cdot r_p}{K \sqrt{\pi} \cdot \arctg \frac{2 \sqrt{a \tau}}{r_p}} \]

The calculation data of distribution of the axial and radial increase of temperature for a bismuth ion beam with a current of 20 \( \mu A \) and a diameter of 0.1 mm in the treatment plane of the target made of titanium, being at room temperature, with formation of the groove with a depth of 0.02 mm are presented in Fig. 1 and Fig. 2.

Figure 1 shows the temperature distribution graphs in depth for a titanium substrate at normal (solid line) and equilibrium (dotted line) distribution of the current density of a bismuth ion beam with the same total power. The comparison shows that in the case of a normal distribution of the ion current density, heat flux \( q \) increases by a factor of two (law \( 2\sigma \)) and, accordingly, the temperature increases in the beam impact zone.

Figure 2 shows the radial temperature dependence of the beam current density for a titanium substrate at normal (solid line) and equilibrium (dotted line) current density distribution of a bismuth ion beam.
Figure 1. The temperature distribution in depth for titanium at normal current density distribution of a bismuth ion beam (solid line) and at equilibrium current density of the beam (dotted line).

Figure 2. The radial temperature distribution for titanium at normal current density distribution of a bismuth ion beam (solid line) and at equilibrium current density distribution of the beam (dotted line).

Figure 3 shows the radial dependence of temperature at normal current distribution of a gold ion beam with a current of 2.5 pA and a diameter of 100 nm when forming the groove with a depth of 40 nm in the treatment plane of a substrate made of molybdenum being at room temperature.
Figure 3. The radial temperature distribution for a molybdenum substrate at normal current density distribution of a gold ion beam.

4. Conclusion
The conducted studies have shown that with the limiting current beam characteristics (the beam current limitation is determined by the volume charge) and the exposure time providing the required depth of the groove, the temperature increase in the irradiation zone on the substrate is insignificant and cannot lead to a property change of the processed material. Thus, the method of forming regular micro- and nanoreliefs by means of a fine-focused heavy ion beam can be referred to the "cold-working" type of material processing.

References
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