Research of the temperature fields influence on the stress state of internal cylindrical surfaces modified by magnetron sputtering

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Abstract. For material selection of protective metal coating, deposited on the products’ surface with cylindrical symmetry by magnetron sputtering and exposed to intense heat loads during pulsed operation mode, it was executed numerical simulation of the temperature fields and the stress state caused by pressure and uneven temperature distribution. It was determined a coating’s material satisfying the minimum of internal stresses, which is one of the main criteria of their service life. Based on the calculation results titanium provides the maximum reduction in the internal stress while the usage of molybdenum as a coatings’ material leads to the greatest decrease of pulsed temperature impact to the binary “steel–coating” systems with cylindrical symmetry.

1. Introduction
Numerical modeling of the temperature and stress fields in cable articles [1], heat pipes [2], thermal tubes [3] and shells [4] with cylindrical symmetry may be used at designing the thermal–stress modes for control systems. Formation of thermally induced residual stress due to plastic deformation during plasma etching step of the symmetric RF–MEMS fabrication process was explained and modeled using the Bauschinger effect [5]. There are several investigations reporting about residual stress evaluation on a cylindrical surface by use of the conventional X-ray stress measuring technique [6, 7].

Thus, the problem relevance of the temperature decrease and, as a result, thermal–stresses reduction in various fields of manufacturing industry caused by the wide usage of products with cylindrical symmetry, operating under dynamically changing temperature fields and aggressive environments. Surface modification of products for their service life extension by physical and chemical methods of thin coatings forming is one of the possible ways to solve this problem. Data on the temperature and internal stresses distribution require for determining the optimal coatings’ composition. Simulations of the temperature fields, radial and tangential stresses in the binary “steel...
coating” systems with cylindrical symmetry was conducted. Titanium, molybdenum, tungsten and tantalum were used as coating materials for calculations.

2. Method of the temperature fields computation in systems with cylindrical symmetry

To determine the temperature fields we used the equation of thermal conductivity. As the temperature changes can reach 1000 K during heating, we cannot neglect the thermal parameters’ dependence from the temperature; therefore the heat equation was solved numerically. All thermo–physical parameters of material were introduced as a piecewise linear function at intervals of 100 K, so it was used an implicit finite–difference scheme for the heat equation solution. To solve the heat equation the following initial and boundary conditions were used:

\[
\begin{align*}
\varepsilon_1 \sigma (T_I^4 - T_{gas1}^4) + \alpha_1 (T_I - T_{gas1}) &= \lambda_1 \frac{\partial T}{\partial r_{r = r_1}} + Q(r, t) \\
T_{p1}(r = R_{2+0}) &= T_2(r = R_{2+0}); -\lambda_2 \frac{\partial T_1}{\partial r} &= -\lambda_2 \frac{\partial T_2}{\partial r}
\end{align*}
\]

Here \(T_I\) is the temperature of a sample surface, from influence of a thermal flow; \(T_{gas1}\) is the gas temperature, from a heated surface; \(T_N\) is the surface temperature, from the outside, not subjected to thermal influence; \(T_{gas2}\) is the gas temperature, from the outside, not subjected to thermal influence; \(\varepsilon\) is a surface blackness degree; \(\sigma\) is a Stephan–Boltzmann’s constant; \(\alpha\) is the coefficient of proportionality in Newton–Rikhman’s equation; \(Q(x, t)\) is the heat flow.

The first equation from system (1) reflects the radiation and convection heat transfer on the internal cylindrical surface with coating. The second equation relates to the interface between the coating and matrix. This boundary condition introduces the continuity of the temperature distribution and the heat flow equality on the coatings’ border from matrix [8]. As initial conditions, the temperature is evenly distributed radially and is equal to 300 K. On the basis of the proposed calculation method was designed a computer program. Verification of its operation was carried out by comparison of analytical solution for the case of a fixed temperature from the outside and inside of cylinder with the constant thermal parameters. The verification was considered stationary when the temperature distribution did not change over time. As the computation results and the analytical solution show, a relative error has the differences of 0.089 %. To analyze the coatings behavior at the impulse impact of concentrated energy flows within the system with cylindrical symmetry, consider a pipe with internal diameter of 9 mm, the system pressure up to 100 MPa, the gas temperature of 3000 K. Determination of the heat transfer coefficient is performed by the empirical equation (2) at pressures in the range from 100 to 500 MPa:

\[
\alpha_I = 90 \times 4.18 \times 1000 \times (1000 \tau)^{0.8384} \exp(-1.200\tau)
\]

Here \(\tau\) is the pulse duration [9].

Due to substitution of thermo–physical parameters’ dependency from the temperature as the result of pulsed heating process we obtained the following temperature distribution (see figure 1). It was conducted a calculations of the pressure pulsed propagation with value of 100 MPa in a pipe with a diameter of 9 mm, at a gaseous medium temperature of 3000 K and 0.3 ms pulse duration. As calculations show titanium coating with a 10 µm thickness on a steel matrix has a maximum temperature while molybdenum coating has a minimum temperature. To analyze the protective coatings’ application under different conditions, cooling water vapor was calculated in the system with
1000 K vapor temperature. In this case the maximum integral coefficient of heat transfer from the water vapor to the surface takes the value of 104 W/(m²K). As the calculation results indicated the maximum temperature amounted to 618 K for 2 seconds heating duration. The temperature difference between the steel and the coated pipes was 1 K. The temperature distribution profile is completely determined by the matrix thermal conductivity. Analysis of different time intervals indicates that 1 ms impulse duration is the high value of the time range for protective coatings using to reduce the temperature maximum.

![Figure 1](image_url)

**Figure 1.** The temperature distribution through the radial direction of matrix with cylindrical symmetry and internal coating at 3000 K gas temperature, 0.3 ms pulse duration; the dashed line is the coatings’ boundary.

To protect the surfaces of steel products with cylindrical symmetry from destruction during its operation at ultrafast pulsed heating and cooling impact from concentrated energy flows, the fields of temperature and internal stresses are the key determining factors. Internal stresses often lead to the mesh cracks formation with followed crumbling and product failure [10].

3. **Method of the internal stress state computation in systems with cylindrical symmetry**

The initial equations we use for internal stress calculation at uneven temperature distribution is the system borrowed from the reference [11]:

\[
\begin{align*}
\varepsilon_r &= \frac{1}{E_T} (\sigma - \nu_T \sigma_r) + \varepsilon_{T,r} \\
\varepsilon_\tau &= \frac{1}{E_T} (\sigma - \nu \sigma_\tau) + \varepsilon_{T,\tau}
\end{align*}
\]

\[\varepsilon_{T,\tau} = \int_{r_0}^{r} \alpha_T dT\] (3)

Here \(\varepsilon_r\) and \(\varepsilon_\tau\) are the relative deformations in the radial and tangential directions correspondently; \(E_T\) is the Young's modulus (index indicating the parameter dependence from the
temperature); \( \sigma_r \) and \( \sigma_t \) are the radial and tangential stresses correspondently; \( \nu_T \) is the Poisson's coefficient; \( \varepsilon_{r,T} \) is the deformation caused by thermal expansion; \( \alpha_T \) is the linear expansion coefficient and \( T \) is the temperature.

To solve the system of equations (3) this paper proposes the following method. We use a combination of analytical and numerical scheme and divide the system by finite differences method on the radial sections so that it can be considered within these areas the physical and mechanical properties \( (E_T, \nu_T, \alpha_T) \) do not depend on temperature. As a result of integration with using the boundary conditions we obtain:

\[
\sigma_r = \left( P_0 - \frac{r_2}{r_2 - r_1} \right) (P_0 - \frac{aE}{(1 - \nu)r_2^2} \int \tau_T dr) - \frac{aE}{(1 - \nu)r_2^2} \int \tau_T dr + \frac{aE}{r_2} \int \tau_T dr \\
+ \frac{1}{r} \left( \frac{r_2}{r_2 - r_1} \right) \left[ P_0 - \frac{aE}{(1 - \nu)r_2^2} \int \tau_T dr \right] + \frac{aE}{(1 - \nu)} \int \tau_T dr \\
\sigma_t = \left( P_0 - \frac{r_2}{r_2 - r_1} \right) (P_0 - \frac{aE}{(1 - \nu)r_2^2} \int \tau_T dr) - \frac{aE}{(1 - \nu)r_2^2} \int \tau_T dr + \frac{aE}{r_2} \int \tau_T dr \\
+ \frac{1}{r} \left( \frac{r_2}{r_2 - r_1} \right) \left[ P_0 - \frac{aE}{(1 - \nu)r_2^2} \int \tau_T dr \right] - \frac{aE}{(1 - \nu)} \int \tau_T dr \\
+ P_0 - \frac{r_2}{r_2 - r_1} \left( P_0 - \frac{aE}{(1 - \nu)r_2^2} \int \tau_T dr \right)
\]  

Here \( P_0 \) is pressure inside the pipe, \( r_1 \) is the internal radius and \( r_2 \) is the external radius.

4. Results and discussion

The initial data we use for calculations are the following values: the pipes’ diameter of 9 mm, at a temperature 3000 K of the gaseous medium, the pressure of 100 MPa, 0.3 ms pulse duration and 10 \( \mu \)m coating thickness at a different coatings composition. In accordance with calculation results (see figure 2), stresses are composed of two competitive components in the radial direction (4): the first type caused by the pressure inside the cylinder (compressive mechanical stresses) and the second induced by the temperature (stretching stresses). Thus, the resulting stress is decreased. With this type of mechanical loading stresses are determinative, in addition, they considerably less than a tensile strength of material and cannot lead to the cylinder destruction. Calculation of tangential (stretching) stresses show its reduction by products’ with protective coatings compared with the unmodified steel parts (see figure 3). It has a great importance for increasing the products lifetime because the tangential stresses are responsible for the mesh cracks formation on the surface of parts with followed crumbling and product failure. Reducing the maximum of tangential stresses is determined by thermo–physical properties of the coatings’ material. Based on the calculation results titanium provides the maximum reduction of the internal stress while the usage of molybdenum as a coating leads to the greatest decrease of the pulsed temperature impact in the binary “steel–coating” system with cylindrical symmetry.
Figure 2. The radial stresses distribution through the matrix with cylindrical symmetry and internal coating at 3000 K gas temperature, pressure of 100 MPa, 0.3 ms pulse duration; the dashed line is the coatings’ boundary.

Figure 3. The tangential stresses distribution through the matrix with cylindrical symmetry and internal coating at 3000 K gas temperature, pressure of 100 MPa, 0.3 ms pulse duration; the dashed line is the coatings’ boundary.
5. Conclusion
Analysis of different time intervals indicates that 1 ms impulse duration is the high value of the time range for protective coatings usage to reduce the temperature maximum. The greatest decrease of the temperature maximum provides by molybdenum coatings that reveals the optimal thermo–physical properties in the case when temperature is decisive for the products’ service life (e.g., corrosion protection [12]). Tangential stresses take the maximum value and can reach 250 MPa under pulsed heating impact on the products with cylindrical symmetry. Application of protective coatings formed by physical and chemical methods (including magnetron sputtering) reduces tangential stresses up to 125 MPa that is quite significant for their service life.

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