Stresses in the material with multilayered coating under impulse thermal loading

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Abstract. The two-dimensional model of mechanical behavior of the specimen with multi layered coating is formulated. The parametric analysis was carried out for various types of boundary conditions. Stress intensity depending on time was studied. The influence of impulse parameters on the temperature and stresses was investigated. It was revealed that radiation heat losses reduces the action of external loading.

1. Introduction
Multilayered materials and coatings are attractive for many applications: in optics and electronics, in semiconductorand metallurgy industries. The combination of layers with different properties allows obtaining unique materials. It relates to the coatings based on TiN and TiC and their solutions [1, 2] and to the coating forming from AlN [3]. Immediate detailed investigation of the structure and properties of multilayered coatings is quite problematically [4-6].

Nowadays, finite-element software are used extensively for engineering calculations. For example, COMSOL, ANSYS, NASTRAN and etc. are widely-distributed. Investigators and developers assert that one can solve any problems and construct predictive models with the help of multiphysical software. In practice it is provided to be changing the objects by some analogies reflecting physical situation quite approximately. We analyze as an example enough simple problem on strain-stressed state calculation of material with multi layered coating in two-dimensional formulation. Using the model presented in [7], we can carry out a series of numerical experiment and obtain the coating with some distributions phases and elements, and residual stresses in the coating. Now it is necessary to investigate the behavior of this coating at the exploitation conditions. We use here COMSOL MULTIPHYSICS [8].

2. Problem formulation
It is assumed that multilayered coating was deposited on iron substrate with the thickness $L = 1$ μm, and the high is $H = 3$ μm. The coating contain the layers from aluminum and titanium nitrides; the thickness of each layer is $h = 0.25$ μm (Figure 1).

The impulse heat flux acts from external sin of the coating. Lateral surfaces of specimen are insulated.

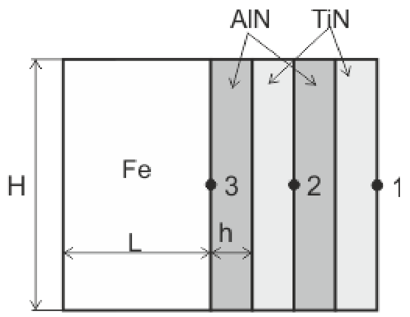


Figure 1. Illustration to the problem formulation.

Mathematical model will include heat and mechanical parts. Temperature field follows from thermal conductivity equation with thermal physical properties different for each layer and for substrate

$$(c\rho)_i \frac{\partial T_i}{\partial t} = \lambda_i \left(\frac{\partial^2 T_i}{\partial x^2} + \frac{\partial^2 T_i}{\partial y^2} \right); \quad \text{i=1…5,} \tag{1}$$

and boundary and initial conditions:

$$\left. \frac{\partial T_1}{\partial y} \right|_{x=0} = 0;$$

$$\left. \frac{\partial T_i}{\partial x} \right|_{y=0} = 0; \quad \left. \frac{\partial T_i}{\partial x} \right|_{y=H} = 0; \; \text{i=1…5}$$

$$\lambda_j \left. \frac{\partial T_j}{\partial y} \right|_{x=L+i\cdot h} = \lambda_{j+1} \left. \frac{\partial T_{j+1}}{\partial y} \right|_{x=L+(j+1)\cdot h}; \; \text{j=1…4}$$

$$T_i = T_{i+1};$$

$$-\lambda_4 \left. \frac{\partial T_4}{\partial y} \right|_{x=L+4\cdot h} = q(t),$$

where

$$q(t) = q_0 f(t) + \sigma\varepsilon(T_0^4 - T^4), \quad f(t) = \begin{cases} 0; \; \sin(at) < b; \\ 1; \; \sin(at) > b, \end{cases}$$

a, b – are some constants.

Practically, for these conditions, thermal conductivity process will as one-dimensional. Mechanical part of the problem is quasistatic thermal elasticity problem. In this case, only two equilibrium equations are used

$$\begin{aligned} &\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0; \\ &\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} = 0, \end{aligned} \tag{2}$$

and it is assumed that specimen is very large in the direction z, that is $\varepsilon_{zz}=0$ and $\sigma_{zz}\neq 0$.

In thermal elasticity theory,

$$\sigma_{kj} = 2\mu\varepsilon_{kj} + \delta_{kj}\left(\lambda\varepsilon_{ll} - 3K\alpha_T\theta_i\right),$$

where θ=$T_i T_0$, i=1…5; λ,μ are Lame coefficients; K is bulk module; $K = \lambda + \frac{2}{3}\mu$. All modules and thermal expansion coefficients are different for different materials (indexes are omotted). Modules connect with technical values by relations

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)};\ \mu = \frac{E}{2(1+\nu)}.$$

In the situation under study, we have

$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x};\ \varepsilon_{yy} = \frac{\partial u_y}{\partial y};\ \varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right),$$

$$\varepsilon_{zz} = 0\,. \tag{3}$$

Hence,

$$\begin{aligned}\sigma_{xx} &= 2\mu\varepsilon_{xx} + \lambda(\varepsilon_{xx} + \varepsilon_{yy}) - 3K\alpha_T\theta_i\\ \sigma_{yy} &= 2\mu\varepsilon_{yy} + \lambda(\varepsilon_{xx} + \varepsilon_{yy}) - 3K\alpha_T\theta_i\\ \sigma_{zz} &= \lambda(\varepsilon_{xx} + \varepsilon_{yy}) - 3K\alpha_T\theta_i\\ \sigma_{xy} &= 2\mu\varepsilon_{xy}\,.\end{aligned} \tag{4}$$

Substituting (4) in (2) and taking into account (3) we come to the equations in displacements

$$\begin{aligned}&\mu_i\nabla^2 u_x + (\lambda_i + \mu_i)\frac{\partial}{\partial x}\left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y}\right) - 3K_i\alpha_{Ti}\frac{\partial\theta_i}{\partial x} = 0;\\ &\mu_i\nabla^2 u_y + (\lambda_i + \mu_i)\frac{\partial}{\partial y}\left(\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y}\right) - 3K_i\alpha_{Ti}\frac{\partial\theta_i}{\partial y} = 0\,,\end{aligned} \tag{5}$$

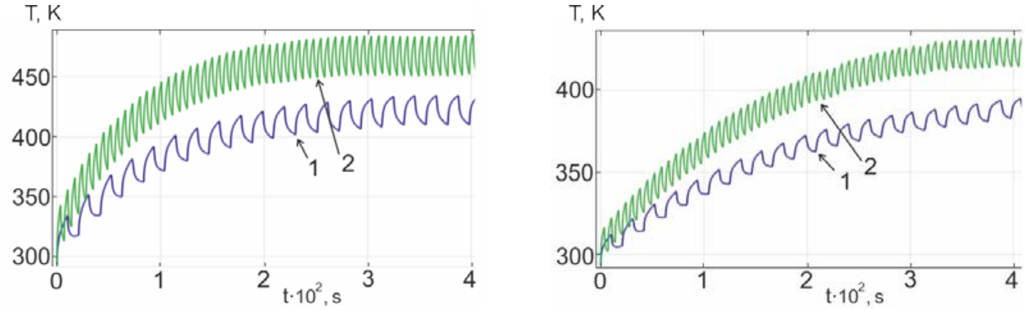
Note that possible dependencies on spatial coordinate for the properties near the interfaces are not taken into account in (5). Boundary conditions in interfaces between layers are ideal, that is the stresses σ_{xx} for layers and displacements u_x are continuous. Specimen is free on external mechanical loading. Initial stresses and strains are zero. After solution of the problem, stresses and strains are determined using (3) and (4). Physical parameters used in calculations are presented in Table 1 drawn up based on the data from [9].

Table 1. Properties of chemical substances.

Parameter	**Fe**	**AlN**	**TiN**	**UM**
λ	80.1	36.2	36.2	W/(m·K)
ρ	7.87	4.93	4.93	$\cdot 10^3$, kg/m^3
C_p	25.14	34.23	34.23	J/(mol·K)
m	55.84	61.8	61.8	$\cdot 10^{-3}$, kg/mol
E	190	326	326	GPa
ν	0.28	0.29	0.29	
α_T	4	3.2	3.2	$\cdot 10^{-6}$, K^{-1}

3. Results

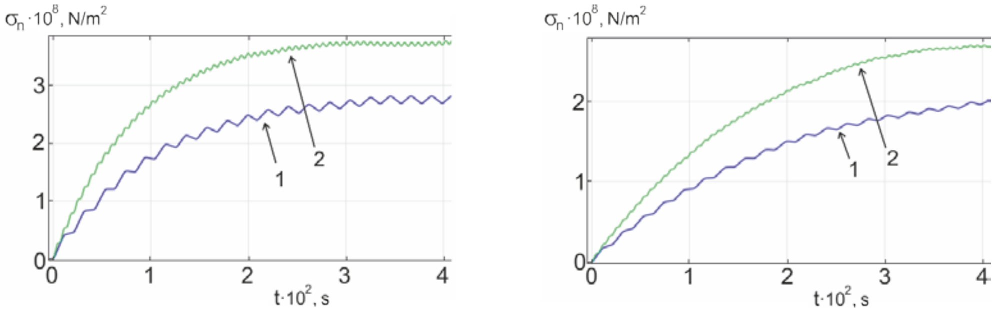
Calculations show that temperature distribution and stresses depend basically on duration of external impulse (area of the action) and on its amplitude. Temperature versus time is presented in Figure 2a and Figure 2b in the point number 2 Figure 1 for uniform and for non uniform heat fluxes. With impulse duration decrease and amplitude growth, maximal temperature naturally rises. Maximal temperature growths more quickly for uniform heating.



a b

Figure 2. Dependence of the temperature of the point of time for the uniform (a) and nonuniform (b) of boundary conditions 1 – a = 0.3, $q_0 = 1\cdot105$; 2 – a = 0.9, $q_0 = 2\cdot105$.

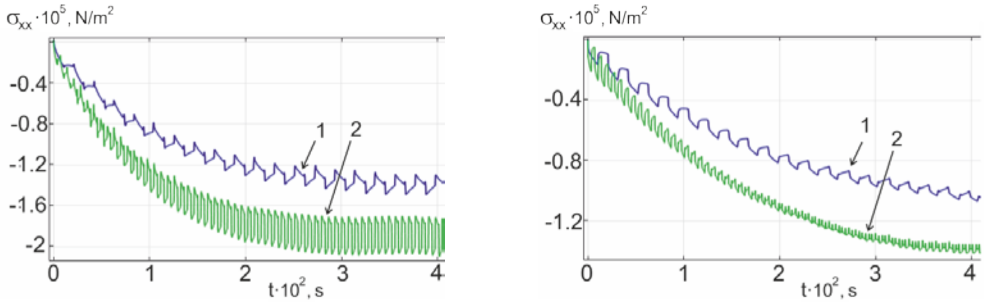
Stresses follow temperature. Impulse duration and its amplitude affect stresses by similarly way. Stress intensity is shown from Figure 3a, b). The values of stresses for presented parameters do not achieve strength limit. Heat losses lead to two-dimensional symmetrical picture of the process development.



a b

Figure 3. Dependence of the intensity of stresses at the point of time for the uniform (a) and no uniform (b) of boundary conditions 1 – a = 0.3, $q_0 = 1\cdot105$; 2 – a = 0.9, $q_0 = 2\cdot105$.

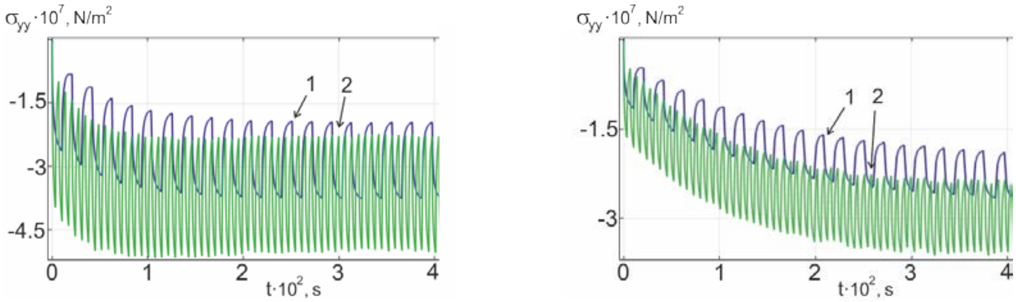
Stress tensor component σ_{xx} growths with time (Figure 4). For uniform heating, difference in maximal and minimal values of stresses during one impulse growths with time, and then it stay constant. For no uniform heating, difference in maximal and minimal values of stresses is small.



a B

Figure 4. Dependence of the stress σ_{xx} at the point of time for the uniform (a) and no uniform (b) of boundary conditions. 1 – a = 0.3, $q_0 = 1\cdot105$; 2 – a = 0.9, $q_0 = 2\cdot105$.

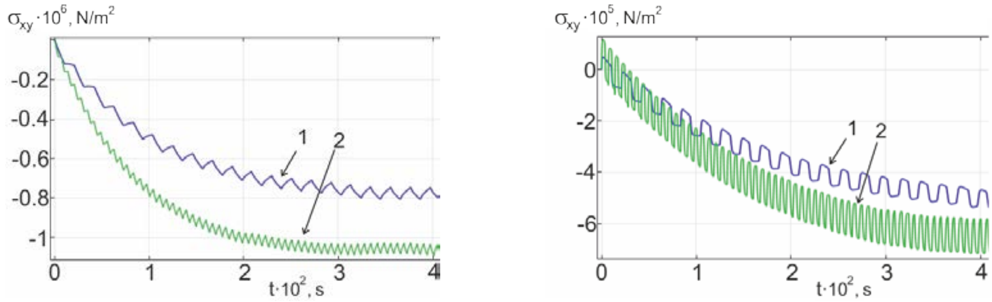
Stress tensor component σ_{yy} changes in a different way. Its value is more in two step then σ_{xx}. (Figure 5a, b). For uniform heating, stationary state (when difference in maximal and minimal values of σ_{yy} does not change) set enough quickly (during 100 s). For no uniform heating, we come to no stationary process.



a b

Figure 5. Dependence of the stress σ_{yy} at the point of time for the uniform (a) and nonuniform (b) of boundary conditions. 1 – a = 0.3, $q_0 = 1{\cdot}10^5$; 2 – a = 0.9, $q_0 = 2{\cdot}10^5$.

In contrast to stresses σ_{yy} and σ_{xx} , maximal value of tangential stresses is higher for no uniform heating then for uniform one (Figure 6a, b).



a b

Figure 6. Dependence of the stress σxy at the point of time for the uniform (a) and nonuniform (b) of boundary conditions. 1 – a = 0.3, q_0 = 1·105; 2 – a = 0.9, q_0 = 2·105.

In (Figure 7a, b) shows the temperature distribution in the sample for some time for the cases of uniform distribution of heat flux along the boundary (a) and for no uniform one (b). For second case, maximal temperature reaches naturally in symmetry axis.

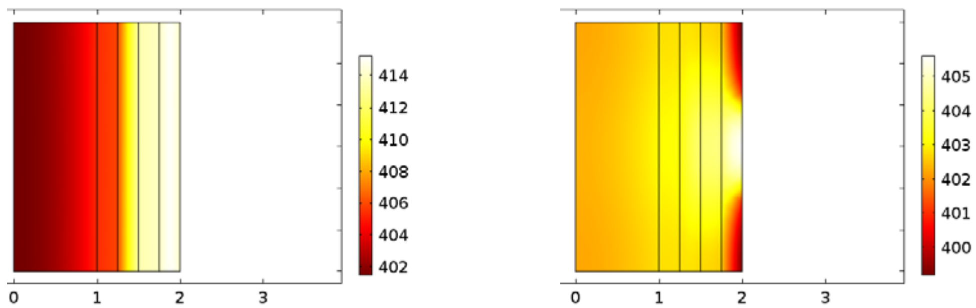


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Figure 7. Temperature distribution in the sample at time t = 250 s

4. Conclusion

Thus, in this paper, on the base of two-dimensional thermal elasticity model the investigation of stresses and temperature evolution in the specimen with multilayered coating was investigated for different parameters of the heating. In quasi static formulation, stresses follow temperature: the temperature growth with the heating parameters leads to stresses evaluation. It was marked that strength limit is not achieved for given parameter set. For more realistic picture, the model should take into consideration the no uniform concentration distribution had been obtained in real and numerical experiment with coating deposition.

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