Modeling of thermal stresses in inorganic matrix composite plates based on the asymptotic theory

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Abstract. A mathematical model has been developed for calculating a temperature non-stationary field and thermal stresses in thin multilayer plates of fabric composite materials on an inorganic matrix based on an alum-chromophosphate binder. The model allows to take into account changes in the microstructure in the matrix and composite fibers during high-temperature heating, taking into account the physical and chemical transformations occurring in them, as well as to calculate thermal stresses in thin plates from the tissue inorganic composite taking into account the kinetics of changes in the characteristics of composites during heating. Methods of multiscale homogenization and finite element modeling of microstresses in periodic cells were used to calculate the characteristics of the inorganic composite, and the method of asymptotic averaging was used to calculate the stresses in the plates. Some results of numerical simulation of the change in stresses in the composite plate during heating are given.

1. Introduction

Composite materials based on inorganic binders (phosphate, alumino-phosphate, chromo-phosphate, magnesium-phosphate, alum-chromophosphate (ACP)) are a promising class of structural materials for the creation of heat-loaded structures [1-3], consisting of oxide ceramic-fibers, and ACP with the addition of dispersed ceramic fillers. At high temperatures up to 1500 °C, complex phase transformations occur in the matrix and fibers of such composite materials, leading to non-monotonous irreversible changes in all the thermal mechanical properties of the material. A multiscale model of the internal structure of the alum-chromophosphate composite was proposed in [3,4]. The purpose of this paper is to construct a mathematical model for calculating thermal stresses in thin composite plates based on transformations based on a multiscale structural model.

2. The mathematical formulation of the problem of calculating the thermal stresses in a composite plate under unsteady heating

Consider for a multilayer plate of inorganic composite a 3-dimensional problem of the linear theory of thermoelasticity, which is written in a dimensionless form as follows [5]

\[
\nabla \sigma_{ij} = 0; \quad \frac{C}{\kappa^2} \partial_t \theta = -\nabla q_i; \\
\sigma_{ij} = C_{ijkl} (\epsilon_{kl} - \epsilon_{kl}^T); \quad q_i = -\lambda_{ij} g_{ij};
\]

(1)
\[ \varepsilon_{ij} = \frac{1}{2} (\nabla_i u_j + \nabla_j u_i); \quad g_j = \nabla_j \theta; \]
\[ \Sigma_{33} : \sigma_{33} = -\kappa^3 p_{\pm} \delta_{33}, \quad q_3 = \pm q_{\pm} \varepsilon_3; \]
\[ \Sigma_T : u_i = u_{i0}, \quad q_i n_i = 0; \]

In system (1), the following are indicated: \( \nabla_j = \partial / \partial x_j \) - the differentiation operator by dimensionless Cartesian coordinates, \( x_i = \tilde{x}_i / L \), \( L \) - plate length, \( h \) - its thickness, \( \kappa = h / L \), \( p_{\pm} \) - pressure, \( q_{0\pm} \) - heat flux on the outer and inner surfaces of the plate \( \Sigma_{33} \) (their equation has the form \( x_3 = \pm \kappa / 2 \)), \( u_{\pm i} \) - given components of the displacement vector on the ends of the plate \( \Sigma_T \), the ends are assumed to be heat insulated. The indices: \( i, j, k, l = 1, 2, 3 \) and large: \( I, J, K \ldots \) - take the values 1,2. Equations (1) also denote: \( \varepsilon_{ij} \) - the components of the small strain tensor, \( \varepsilon_{kl}^T = \alpha_{kl} \Delta \theta \) - the components of the thermal strain tensor, which are functions of the temperature difference \( \Delta \theta = \theta - \theta_0 \), where \( \theta_0 \) is the initial temperature, \( \alpha_{kl} \) are the components of the thermal expansion tensor. The components of the tensor of the modulus of elasticity \( C_{ijkl} \), thermal conductivity \( \lambda_{ij} \), thermal deformation \( \varepsilon_{kl}^T \), as well as the mass heat capacity \( C = \rho c / F_{o0} \) are variables, they depend on the variable phase composition of the plate material.

The following assumptions are made in system (1): 1) the parameter \( \kappa \) is small \( \kappa \ll 1 \), 2) the pressure on the outer and inner surfaces of the plate has the third order of smallness \( O(\kappa^3) \) (i.e. \( \sigma_{33} = -\kappa^3 p_{\pm} \)), 2) the heating time is not too large, in the sense that the Fourier criterion \( F_0 = \lambda_{0}^0 t_0 / \rho_o c_o L^2 \) of the process heating has one order of smallness with \( \kappa^2 \) (i.e., \( F_0 = \kappa^2 F_{o0} \)), where the \( F_{o0} \) number is of the order of 1: \( F_{o0} = O(1) \); 3) pressure \( p_{\pm} \) and heat flux \( q_{0\pm} \) vary little over distances of the order of \( h \).

3. Multi-level model of inorganic composite material at high temperatures

Composite materials based on ACP according to the general methodology for modeling composites [6] will be considered as a multi-level structure consisting of 4 structural levels. The first level of this structure is formed by the periodicity cells N 1 (PC1), which consist of 2 elements: oxide fibers and the matrix ACP, \( \varphi_f, \varphi_m \) — their volume concentrations, \( \varphi_f + \varphi_m = 1 \). In oxide fibers, phase transformations occur during heating: amorphous ("a") and crystalline ("l"), \( \varphi_a, \varphi_l \) - their concentration, related by the ratio \( \varphi_a + \varphi_l = 1 \).

At the 2nd level, the matrix is considered as ACP (polymer) with a filler in the form of ceramic particles based on chromium and aluminum oxides. At the 3rd level, ACP is considered as PC3, containing two phases, each of which corresponds to the transformation of the polymer along the aluminum and chromium chain, respectively, we denote the concentrations of the aluminum and chromium chains of phase transformations: \( \varphi_{Al}, \varphi_{Cr} \), and \( \varphi_{Al} + \varphi_{Cr} = 1 \). For the 4th level PC, we introduce the following notation: \( \varphi_2 \) - volume concentration of polymer P-phase, \( \varphi_3 \) - metaphosphate
M-phase, $\varphi_4$ - orthophosphate O-phase, $\varphi_5$ - ceramic C-phase, $\varphi_6$ - concentration of gas g-phase. These phase concentrations are related by $\varphi_2 + \varphi_3 + \varphi_4 + \varphi_5 + \varphi_6 = 1$

The system of equations of continuity for the 6th environment has the following form:

$$\rho_2 \frac{\partial \varphi_2}{\partial t} = -J_2, \quad \rho_3 \frac{\partial \varphi_3}{\partial t} = -J_3(1 - \Gamma_2) - J_3, \quad \rho_4 \frac{\partial \varphi_4}{\partial t} = J_3 - J_4,$$

$$\rho_5 \frac{\partial \varphi_5}{\partial t} = J_4(1 - \Gamma_5), \quad \rho_6 \frac{\partial \varphi_6}{\partial t} = \nabla \varphi_6 \rho_6 \tilde{V}_6 = J_4 \Gamma_5,$$

where are marked: $J_i = J_i^0 \varphi_i \exp\left(-\frac{E_{Ai}}{R \theta(t)}\right)$ - mass velocities of phase transformations, $\Gamma_i$ - gasification coefficients, $\rho_i$ - phase density, $E_{Ai}$ - activation energy, $J_i^0$ - pre-exponential factors characterizing the rate of phase transformations, $R$ - gas constant, $\tilde{V}_6$ - filtration vector of gas phases in pores.

4. A model for the elastic properties of the matrix under high temperature

The modulus of elasticity of the inorganic matrix is calculated by the mixture formula

$$E_m = E_{m-Al} \varphi_{Al} + E_{m-Cr} \varphi_{Cr},$$

where $E_{m-Al}$ and $E_{m-Cr}$ - the elastic moduli of the aluminum-containing and chromium-containing parts of the matrix

$$E_{m-Al} = \left( \frac{1 - S_C}{E_1} + \frac{(S_C - S_O)}{E_2} \right) \left( \frac{S_O - S_M}{E_3} \right)^{-1} \left( \frac{S_M - S_P}{E_4} \right) + \frac{S_P}{E_5},$$

$$\varphi_3 = 1 - S_C^3, \quad \varphi_4 = S_C^3 - S_O^3, \quad \varphi_5 = S_O^3 - S_M^3, \quad \varphi_2 = S_M^3 - S_P^3, \quad \varphi_6 = S_P^3,$$

and $E_i$ - the moduli of elasticity of the matrix phases $i = 1 \ldots 6$. For the modulus of elasticity of the C phase at high temperatures, we adopt the following model:

$$E_C = E_C \left(1 - a_0 \left( (\theta - \theta_b) / \theta_b \right)^n \right),$$

where $n, a_0$ are the constants.

5. Model changes in phase composition and elastic properties of oxide fibers under high temperatures

The change in the volume concentration of the “amorphous” phase of quartz fibers is described by the equations:

$$\rho_a \frac{\partial \varphi_a}{\partial t} = -J_a, \quad J_a = J_a^0 \varphi_a \exp\left(-\frac{E_{Aa}}{R \theta(t)}\right),$$

where: $\rho_a$ is the density of the amorphous phase, $E_{Aa}$ is the activation energy of the amorphous phase, $J_a^0$ is the preexponential factor.

The change in the elastic modulus $E_f$ of oxide fibers during heating is determined by two factors:
1) a change in the elastic properties of the fiber in the amorphous state at relatively low temperatures;
2) physical and chemical processes of crystallization at high temperatures. The first factor causes a
reversible change in the elastic modulus $E_f$ of the fibers, the second leads to irreversible changes after cooling.

$$E_f = \left( \frac{1 - S_f}{E_i} + \frac{S_f}{E_2} \right)^{-1}, \quad E_i = E_i, \quad E_2 = (1 - S_f) E_i + S_f E_a, \quad \varphi_i = (1 - S_f^3); \quad \varphi_i = S_f^3 \quad (6)$$

Here $E_i, E_a$ are the elastic moduli of the fiber phases.

To calculate the effective elastic characteristics of PC on the 1st and 2nd levels, a finite-element method for solving problems on periodicity cells was used [7, 8].

6. Effective elastic characteristics of the textile composite

Modern reinforcing filaments consist of a large number of fibers, which are also interconnected by a matrix. To calculate the components of the tensors of the elastic moduli of the threads $C^{(a)}_{ijkl}$, we use the model [9]. To determine the components of the tensor of effective elastic moduli of a composite $C_{ipq}$, we use the solution of a series of local problems $L_{pq}$ on a periodicity cell. These modules $C_{ipq}(E_f, E_m)$ depend on the elastic moduli of the matrix and fibers, taking into account (3) and (6), this dependence is possible as a function of the phase concentrations $C_{ipq}(\varphi_i, E_i)$.

![Figure 1](image)

**Figure 1.** Distribution of the elastic modulus of the matrix and fiber (dimensionless values) across the plate thickness (in cross section $x = 0.25$) of the inorganic composite for two points in time $t_2$ and $t_4$ of non-stationary heating

7. Method for Solving Problem (1)

To solve problem (1), the method of asymptotic expansions was used, with which explicit analytical formulas were found for the stresses in an inorganic composite plate under bending pressure and uneven heating.

$$\sigma_{11} = \frac{C^{(0)}_{1111} \Delta p}{24 \kappa^2 D_{11}} x(x - 1),$$
\[
\sigma_{j3} = \frac{\Delta p}{\kappa D_{11}} (x - 1/2) \left\{ \xi C_{1111}^{(0)} \right\}_\xi, \\
\{ f \}_\xi = \int_{-0.5}^{0.5} (f - f) d\xi 
\]

(7)

\[
\sigma_{33} = -\left( \bar{p}_- + \Delta \bar{p} (\xi + 0.5) - \frac{\Delta \bar{p}}{D_{11}} \left\{ \xi C_{1111}^{(0)} \right\}_\xi \right), \quad \xi < f >= \int_{-0.5}^{0.5} f d\xi 
\]

Here \( D_{11} = \left< \xi^2 C_{1111}^{(0)} \right> \) is the flexural rigidity of the plate, and also denoted by: \( C_{\mu 11}^{(0)} = C_{\mu 11} - C_{\mu 33} C_{3333}^{-1} C_{3311} \), \( \Delta \bar{p} = \kappa^3 \Delta p \), \( \bar{p}_- = \kappa^3 p_- \), \( \Delta p = p_+ - p_- \), \( \xi = x_3 / \kappa \).

Figure 1 shows the graphs of the distribution of the dependence of the elastic modulus \( E_f, E_m \) of the fibers and the matrix in the composite across the thickness of the plate with uneven heating.

A feature of the elastic modulus of an ACP matrix is the increase in its values in the temperature range from 600 to 1100 °C, which is associated with higher values of the elastic moduli of the meta- and orthophosphate phases. Figure 2 shows the distributions of the elastic moduli of a fabric composite based on glass fibers and AHFS over the plate thickness during heating. Figure 3 shows the distribution of flexural stress calculated from (7) for several moments of non-stationary heating.

**Figure 2.** Distribution of the components \( C_{ijkl} \) of the elastic modulus tensor (dimensionless values) over the plate thickness in the section \( x_1 = 0.25 \) for the time \( t_4 \) (1-C_{1111}, 2-C_{2222}, 3-C_{1122}, 4-C_{1133}, 5-C_{2323}, 6-C_{1212}).
Figure 3. Flexural stress distribution $\sigma_{11}$ (dimensionless value) across the plate thickness in the cross section of the plate with coordinate $x_1 = 0.25$ for different moments of the dimensionless time $t_i = 1,2,3$ and 4.

8. Conclusions
The developed mathematical model makes it possible to predict the change in time of the stresses in a thin plate of inorganic composites during unsteady uneven heating to high temperatures, taking into account the physical and chemical transformations occurring in them. The results of numerical simulation have shown that due to the complex non-monotonic nature of the temperature dependence of the elastic properties of the inorganic matrix, the stresses in the plate with uneven heating also have a complex, non-monotonic change over time.

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