The algorithm of numerical solution for thermo-viscoelastic model composite material synthesis based on Ni-Al

Yu.A. Chumakov, T.A. Krylova
chya@ispms.ru

Abstract

The model of the synthesis of a composite based on a Ni-Al system with refractory carbide (TiC) particles is suggested. The various multiscale processes are considered in the model. The model takes into account an interaction of mechanical and thermal processes. The change in the structure of the composite is considered in the two-level approach: an evaluation of the stress-strain state of the system, calculation of thermal and concentration fields during the synthesis are conducted at the macrolevel; the effective properties of the composite are determined at the microlevel. The heat release from chemical reactions is determined by solving the problem of the reaction cell. The algorithm for the numerical solution of the problem is proposed.

1 Introduction

Synthesis of composites in the combustion regime [1-3] or in the thermal explosion mode [4-6] has attracted the attention of researchers [7-9]. The external electric and magnetic fields, as well as various types of mechanical loading are usually used to control the synthesis process. However, the exothermic synthesis process is poorly controlled. Therefore, the predictions of the composition and properties of composites, depending on the conditions of synthesis, use mathematical modeling.

The present work represents the evolution of previous investigations [10-13]. In this paper, we propose a model of the synthesis of a multiphase composite from a mixture of metal powders (Ni and Al), including those with additives of refractory inclusions such as titanium carbide TiC under heating conditions combined with loading. Since a change in the structure of the reaction system is possible during the synthesis process, and the macroscopic model is unable to describe the local structural inhomogeneities of the reaction medium, in this work, in order to take into account the influence of the particle size of the reagents, their distribution, formation of the reaction product layer at the particle level and their correlation with the characteristics of the synthesis process is used the two-level approach. The microstructural model of the reaction cell is considered at the microlevel (the level of individual powder particles) to determine the effective properties of the composite and the heat release from chemical reactions. The methods of continuous medium mechanics, the dynamics of multiphase media, the theory of structural macrokinetics and thermodynamics are used at the macro level to determine the characteristics of the solid-phase synthesis process (the field of temperature, component concentration, stress and deformation).

2 PROBLEM FORMULATION

A flat layer of reagent that can be subjected to external thermal heating and mechanical loading is considered to describe the process of synthesis of composite material. In the model we use the following assumptions:
- in the investigated sample a flat layer of the regent of length L_x, width L_y, thickness L_z is considered. The conditions $L_z << L_y$, $L_z << L_x$ are satisfied, which allows us to use the hypothesis of the plane-stressed state of the plate to estimate the mechanical stresses arising in the system; i.e. $\sigma_{zz} = 0$ (rotations are also not taken into account);
- in the energy equation we take into account the work of dissipative forces and interaction of thermal and mechanical processes
- the properties of the composite are effective ones and the properties are calculated based on the sintering theory and dynamics of multiphase media
-the heat release from chemical reactions is determined from the solution of the problem of chemical reaction in the reaction cell.
- To take into account the melting of the components of the system, we use an abrupt specific heat changing in the vicinity of the melting point

$$c_\varepsilon\rho = \begin{cases} (c_\varepsilon\rho)_S + L_m\delta\left(T - T_m\right),\ T <= T_m \\ (c_\varepsilon\rho)_L + L_m\delta\left(T - T_m\right),\ T > T_m \end{cases},$$

where subscripts "s" and "L" refer to the properties of the solid and liquid (molten) material, respectively; T_m is the melting point, L_m is the heat of the phase transition, and δ is the Dirac delta function.
The mathematical formulation of the problem includes the heat conduction equation associated with deformations and containing two types of heat sources - due to a chemical reaction and due to viscous dissipation.

$$\sigma_{ij}\frac{d\varepsilon_{ij}}{dt} + c_\varepsilon\rho\frac{dT}{dt} = \nabla\cdot\lambda_T\nabla T + \sum_{i=1}^{n} Q_i\phi_i\left(\eta, T\right) - 3K\,T\alpha_T\frac{d\varepsilon_{kk}}{dt} \tag{1}$$

where c_ε, ρ and λ_T are the effective heat capacity, density and thermal conductivity coefficient, respectively; T is the temperature, x and y are spatial coordinates, $\varepsilon_{kk} = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$ is the first invariant of strain tensor, α_T is the thermal expansion coefficient, K is the isothermal bulk modulus, σ_{ij} , ε_{ij} are the components of stress and strains tensors, η is the conversion level or the fraction of the reaction product, Q is the heat of the total reaction, $\phi_i(\eta,T)$ is the chemical reaction rate,

$$\frac{\partial ...}{\partial t} + V\cdot\nabla ... \tag{2}$$

To determine the stressed-strain state of plane layer, we consider the problem of the mechanical equilibrium of the plate in the approximation of generalized plane stress state. Therefore, the problem involves the equilibrium equations, rheological relations and boundary conditions corresponding [14].

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0; \quad \frac{\partial \sigma_{yx}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} = 0 \tag{3}$$

We use the Cauchy equations [14]

$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x}; \quad \varepsilon_{yy} = \frac{\partial u_y}{\partial y}; \varepsilon_{xy} = \frac{1}{2}\left(\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y}\right) \tag{4}$$

We assume that the stress tensor is the sum of the elastic and viscous components:

$$\sigma_{ij} = \sigma_{ij}^{e} + \sigma_{ij}^{V}.$$

We use the Duhamel-Neumann relations for "elastic" stresses

$$\sigma_{ij}^{e} = 2\mu \cdot \varepsilon_{ij} + \delta_{ij}\left[\lambda \varepsilon_{kk} - K\omega\right],$$

where

$$\omega = 3\left[\alpha_T (T - T_0) + \sum_{k=1}^{n} \alpha_k \eta_k\right],$$

n is the number of components involved in the reactions; α_k are the coefficients of concentration expansion.
Elastic stress increments are linearly related to the increments of any deformations. Viscous - linearly related to the rates of deformation. By analogy with the previous one, for viscous stresses we have

$$\sigma_{ij}^{V} = 2\mu_V \cdot \dot{\varepsilon}_{ij} + \delta_{ij}\left[\lambda \dot{\varepsilon}_{kk} - 3K\left(\alpha_T \dot{T} + \sum_{k=1}^{n} \alpha_k \dot{\eta}_k\right)\right],$$

where μ_V is the coefficient of viscosity; δ_{ij} is Kronecker symbol.
For the total reaction, we obtain the expression

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + 2\mu_v \dot{\varepsilon}_{ij} + \delta_{ij}\left[\lambda \varepsilon_{kk} + \lambda \dot{\varepsilon}_{kk} - 3K\left\{(\alpha_p - \alpha_r)\eta + (\alpha_p - \alpha_r)\dot{\eta}\right\}\right] \tag{5}$$

The boundary conditions correspond to the character layer loading (tension, compression, shear) and to the conditions of external heating.

$$\begin{gathered} t = 0 : T = T_0, \quad \sigma_{ij} = 0; \ \varepsilon_{ij} = 0 \\ x = 0 : \ -\lambda \frac{\partial T}{\partial x} = \begin{cases} q_0, t \le t_i \\ \alpha\left(T - T_0\right), t > t_i \end{cases}, x = L_x : \ \frac{\partial T}{\partial x} = 0; \\ y = 0 : \ \frac{\partial T}{\partial y} = 0, y = L_y : \ \frac{\partial T}{\partial y} = 0, \end{gathered} \tag{6}$$

where t_i is the heat flux time; q_0 is the heat flow power; and α is the external heat exchange coefficient.
For the case of uniaxial extension, the boundary conditions have the form

$$\begin{aligned} x = 0, \, x = L_x: \quad \sigma_{xx} = P, \;\; \sigma_{yy} = 0, \;\; \sigma_{xy} = 0; \\ y = 0, \;\; y = L_y: \quad \sigma_{xx} = 0, \;\; \sigma_{yy} = 0, \;\; \sigma_{xy} = 0.x \end{aligned} \tag{7}$$

For the case of uniaxial compression, the load was taken with a negative sign. For the pure shear condition we have

$$\begin{aligned} x = 0, \, x = L_x: \quad \sigma_{xx} = P_1, \;\; \sigma_{yy} = 0, \;\; \sigma_{xy} = 0 \\ y = 0, \;\; y = L_y: \quad \sigma_{xx} = 0, \;\; \sigma_{yy} = P_2, \;\; \sigma_{xy} = 0 \end{aligned} \tag{8}$$

where $P_1 = P{\cdot}\cos(\alpha)$, $P_2 = P{\cdot}\sin(\alpha)$, $\mathrm{tg}(\alpha) = L_x/L_y$.

Algorithm of numerical solution

The algorithm for the numerical solution of the problem under investigation was as follows. For the numerical solution of the heat equation (1) finite-difference approximation using the four-point pattern and the splitting scheme by coordinates were used. The finite-difference scheme for (1) has the form

$$\begin{gathered} c_{ij}\rho_{ij}\frac{\tilde{T}_{ij} - \overset{\vee}{T}_{ij}}{dt} = \frac{1}{dx}\left[\frac{\lambda_{i+1j} + \lambda_{ij}}{2}\frac{\tilde{T}_{i+1j} - \tilde{T}_{ij}}{dx} - \frac{\lambda_{ij} + +\lambda_{i-1j}}{2}\frac{\tilde{T}_{ij} - \tilde{T}_{i-1j}}{dx}\right] \\ c_{ij}\rho_{ij}\frac{T_{ij} - \tilde{T}_{ij}}{dt} = \frac{1}{dy}\left[\frac{\lambda_{ij+1} + \lambda_{ij}}{2}\frac{T_{ij+1} - T_{ij}}{dy} - \frac{\lambda_{ij} + \lambda_{ij-1}}{2}\frac{T_{ij} - T_{ij-1}}{dy}\right] + \\ + \overset{\vee}{W}_{ij} - \overset{\vee}{U}_{ij} + \sum_{i=1}^{n} Q_i \phi\left(\overset{\vee}{\eta}_{ij}, \overset{\vee}{T}_{ij}\right) \end{gathered} \tag{9}$$

where

$$W = \sigma_{ij}\frac{\partial \varepsilon_{ij}}{\partial t}, U = 3K T \alpha_T \frac{\partial \varepsilon_{kk}}{\partial t}.$$

The parameters denoted by the symbol "$\vee$" are the values on the previous time layer. Further, the resulting system of linear algebraic equations was solved by a sweep method with initial and boundary conditions (6). The temperature value for each k time layer (T^k_{ij}(x,y)) was used in kinetic equations and rheological relations. To determine the kinetic function of $\phi(\eta$,T) and the total heat release from chemical reactions, a special problem of chemical reaction is solved at the level of the representative volume (reaction cell). The method used to solve the system of differential equations in the model of the reaction cell is analogous to the solution method for the energy equation presented above.
To find the components of the stress tensor σ_{ij} and deformation ε_{ij} we use the Cauchy equation and the deformation rate relations.

$$V_x = \frac{\partial u_x}{\partial t}; V_y = \frac{\partial u_y}{\partial t}; \quad \frac{\partial \varepsilon_{xx}}{\partial t} = \frac{\partial V_x}{\partial x}; \quad \frac{\partial \varepsilon_{yy}}{\partial t} = \frac{\partial V_y}{\partial y}; \frac{\partial \varepsilon_{xy}}{\partial t} = \frac{1}{2}\left(\frac{\partial V_y}{\partial x} + \frac{\partial V_x}{\partial y}\right) \tag{10}$$

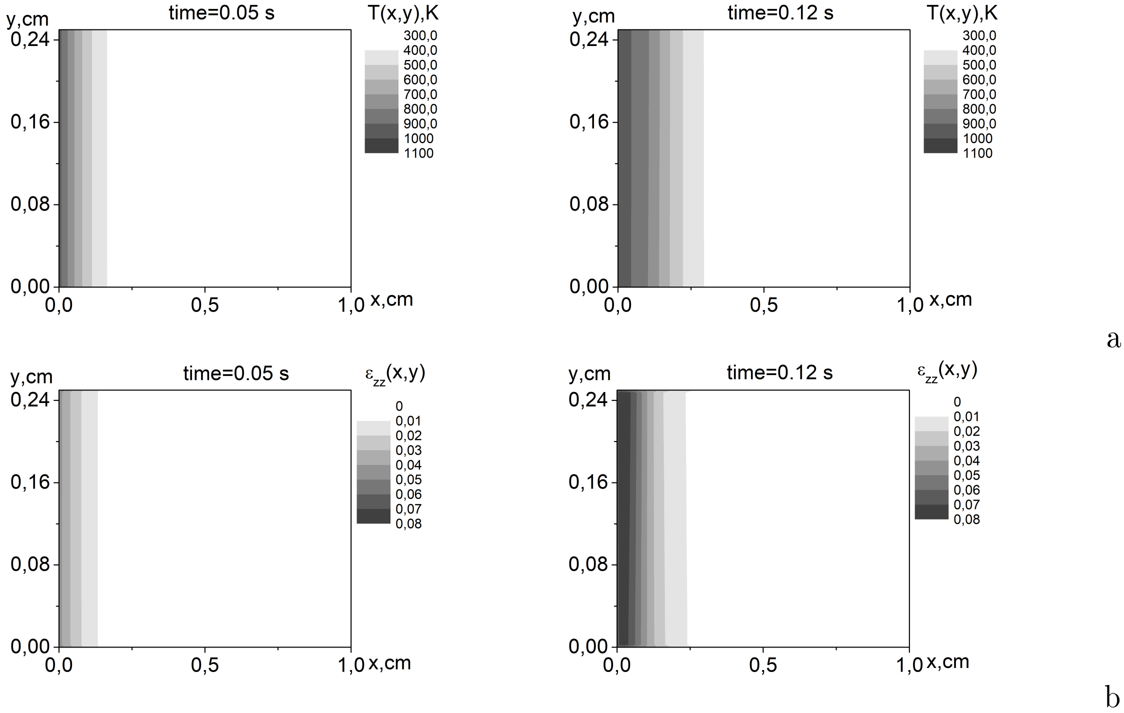

Fig.1. Spatial distributions of the plate temperature (a) and component of strain tensor (b) $q^0 = 10^7 W/m^2, P = 1GPa$

The relations (10) were substituted into the rheological relations (5) and the equilibrium equations (3).Then the differential equations were replaced by difference equations, and the resulting system was solved by the relaxation method. In view of the cumbersomeness, we not represent the founded expressions in the article. The results of calculations based on the proposed algorithm for the viscoelastic Maxwell's body and the case of pure shear are shown in Fig. 1.

Acknowledgements

The work was carried out in the framework of the Fundamental Research Program of the State Academies of Sciences for 2013-2020. Project 23.2.2.

References

[1] Widodo T., Riyadi B., Zhang T., Combustion Synthesis of Ti3Al Composite by Induction Heating,Proceedings of the 3rd Applied Science for Technology Innovation, 2014, 18-23.

[2] Kobashi M., Ichioka D., Kanetake N., Combustion Synthesis of Porous TiC/Ti Composite by a Self-Propagating Mode Materials 2010, 3,3939-3947.

[3] Feng G., Li Zh., Jacob R.J., Yang Y., Wang Y., Zhou Z., Sekuli D.P., Zachariah

M.P., Laser-induced exothermic bonding of carbon fiber/Al composites and TiAl alloys, Materials and Design, 126, 2017, 197-206.

[4] Liang Y., Zhao Q., Han Zh., Zhang Zh., Li X., Ren L., Reaction behavior of TiC/Cu composite via thermal explosion reaction (TE) under Ar and air atmosphere, Corrosion Science, Vol.93, 2015, 283-292.

[5] Shokati A.A., Parvin N., Shokati M., Combustion synthesis of NiAl matrix composite powder reinforced by TiB2 and TiN particulates from Ni-Al-Ti-BN reaction system, Journal of Alloys and Compounds, Vol. 585, 5 February 2014, 637-643.

[6] Liua Ya., Cai X., Sun Zh., Jiao X., Akhtar F., Wang J., Feng P., A novel fabrication strategy for highly porous FeAl/Al2O3 composite by thermal explosion in vacuum, Vacuum, Vol. 149,March 2018,225-230.

[7] Rogachev A.S., Mukasyan A.S. Combustion for Material Synthesis, Taylor Francis Group, 2015.

[8] Moore J.J.,Feng H.J. Combusion synthesis of advanced materials: part I. Reaction parameters,Progress in material science, 1995, Vol.39, 243-273.

[9] Moore J.J.,Feng H.J. Combusion synthesis of advanced materials: Part II: Classification, application and modeling, Progress in material science, 1995. Vol.39, 275-316.

[10] Chumakov Yu.A., Knyazeva A. G. The influence effect of coupling on solid-phase conversion in the plate from composition materials under condition of axial tension and shifting, AIP Conference Proceedings,1623, 2014, 95-98.

[11] Chumakov Yu.A., Knyazeva A.G. Influence of method used for calculating of effective properties on stressed-strain state of composite plate under nonstationary heating, Applied Mechanics and Materials, 756, 2015, 402-407.

[12] Chumakov Yu.A.,Knyazeva A.G. Model of behavior of the viscoelastic system with a melting component under external load, IOP Conf. Series: Materials Science and Engineering,124,012049, 2016.

[13] Chumakov Yu.A., Knyazeva A.G. Porosity evolution during composite synthesis under loading, AIP Conference Proceedings 1909,020028, 2017.

[14] Boley B., Weiner J. Theory of Thermal Stresses, New York, Wiley, 1960.

Yu.A. Chumakov, ISPMS SB RAS, pr. Akademicheskii, 2/4, Tomsk, Russia
T.A. Krylova, ISPMS SB RAS, pr. Akademicheskii, 2/4, Tomsk, Russia