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Influence of Coupling of Thermokinetic and Mechanical Processes on the Composite Synthesis on the Substrate

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Abstract. A coupled mathematical model for the process of a composite synthesis from a powder mixture under laser heating conditions is presented. The model takes into account two phenomena that are neglected in traditional models of surface treatment and 3D technologies. They are the heat transfer-deformation behaviour and heat release in chemical reactions. The formation of composition is described by a simplified reaction scheme that includes the total reaction leading to the formation of hardening particles and the total reaction of matrix formation. The influence of stress work on reaction rates is taken into account. The stress-strain state is described in the quasi-static approximation. As a result, it is shown that coupling of processes of different physical nature is important both for determining composition of the composite and for estimating the associated stresses and strains.

Keywords: coupled model, composite synthesis, associated stresses, controlled mode.

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Introduction

A large number of publications are devoted to process modelling in modern technologies. The authors often repeat each other and use the term "coupled models" unnecessarily. Coupled models should be understood as such models in which the interaction between physical fields is taken into account. There are many examples of coupled models in physics and continuum mechanics. One can mention models of solid-phase combustion theory in which the interaction of heat transfer and chemical reactions is taken into account [1]. Another example is solid-state diffusion models which take into account the interaction of diffusion of atoms and vacancies, the interrelation between diffusion and stresses [2]. However, when modelling the synthesis of new materials, it is of interest to study the stress and strain fields accompanying the synthesis. Together with the external load they influence the kinetic patterns of phase formation through different channels. Despite the fact that term "coupled model" is used in a huge number of publications, there are not many real coupled models. Results of modelling of the temperature field, residual stresses, processes in the melt bath (singled out as an independent object), crystallization in meso-volumes, powder melting in the beam, mechanical behaviour of synthesized

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objects, effective properties from experimentally obtained structural data were presented [3–5]. The aim of this paper is to demonstrate the role of different channels of interaction between processes of different physical nature within the model of synthesis of composite coating on a substrate.

1. General problem formulation

Let us assume that under experimental conditions the mixture of powders from which a coating or a layer of three-dimensional product is formed under the governing of a moving heat source is freely poured on a flat substrate. Chemical reactions may occur in the mixture of powders. Reactions are accompanied by thermal effects. When the melting temperatures are reached the liquid phase appears. Sometimes its appearance in large quantities is undesirable as it may lead to splashing and other negative effects. Therefore, it is convenient to carry out the process in such a way that the area occupied by the liquid phase is small compared to the size of the whole sample or that the proportion of liquid phase anywhere in the sample is negligible. In this case it is possible to neglect melting effects and consider solid-phase processes. Then conventional description of thermokinetic phenomena requires heat conduction equation and kinetic equation:

$$\rho c \frac{\partial T}{\partial t} = -\nabla \cdot J_q + W_{ch} + W_{ext}; \quad (1)$$

$$\frac{d\eta_i}{dt} = \sum_{(k)} \nu_{ik} \Phi_k, \quad (2)$$

where T is the temperature; t is time; ρ is the density; c is the isobaric heat capacity; J_q is the heat flux satisfying the Fourier law $J_q = -\lambda_T \nabla T$; λ_T is the heat transfer coefficient; W_{ch} is the total chemical heat release, $W_{ch} = \sum_{(k)} Q_k \Phi_k$; Q_k is the heat effect of k -reaction (number of which r); Φ_k is the k -th reaction rate; η_i is the concentration of i -component; ν_{ik} is the stoichiometric coefficient of i -component in k -reaction; W_{ext} is the heat source associated with heating by an external energy source (laser, electron beam, electric arc, plasma) which in general case has limited size and it moves along the surface on some specified trajectory.

The boundary conditions at $x = 0$; $x = L_x$; $y = 0$; $y = L_y$ and at the bottom surface of the substrate are related to heat loss by radiation and/or convection. For example, one can write for $x = 0$

$$\lambda_T \frac{\partial T}{\partial x} = \alpha_L (T - T_e) + \sigma_0 \varepsilon_L (T^4 - T_w^4) \quad (3)$$

where T_e is the environment temperature; T_w — is the vacuum chamber wall temperature (if the process is carried out in the chamber); α_L is the heat loss coefficient; ε_L — surface emissivity; σ_0 — Stefan-Boltzmann constant.

When synthesis process is described in detail then properties can depend on temperature, composition and porosity. However, in the vast majority of cases such relationships are unknown. Then one should use some effective values. The influence of these values on the process can be studied in special way [6].

However, considering dynamics of synthesis of new materials the role of the associated mechanical processes is of great interest. These processes are not reflected in (1), (2). In general, in order to take into account the properties of the substrate or surrounding layers and, at the same time, the stress-strain state in the model of controlled coating synthesis three-dimensional heat

conduction equations together with equations of equilibrium are required. However, it leads to cumbersome formulations and it is problematic for parametric studies.

Let us take advantage of the fact that a thin flat substrate together with the coating can be considered as a flat (two-dimensional) object whose thickness is much smaller than its width and length. Then averaging the three-dimensional equations over the thicknesses of the substrate and the coating, one can consider a plane stress state and a two-dimensional problem [7–9]. In this case, the two-dimensional heat conduction equation takes the following form

$$(c_\varepsilon \rho)_{eff} \frac{\partial T}{\partial t} = \lambda_{T,eff} \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \frac{h_R W_{ch} + H}{h_S + h_R} + \frac{W_{ext,eff}}{h_S + h_R} - 3(K\alpha_T)_{eff} T \frac{\partial \varepsilon_{kk}}{\partial t}. \quad (4)$$

Equation (4) contains effective properties (index "eff") that take into account the properties and thicknesses of the powder layer and the substrate [7] as well as two new terms. One of them takes into account heat losses from the surfaces of the substrate and coating:

$$\frac{H}{h_S + h_R} = \frac{\alpha_{eff}}{h_S + h_R} (T - T_0) + \frac{\sigma_0 \varepsilon_{eff}}{h_S + h_R} (T^4 - T_w^4) = \alpha'_{eff} (T - T_0) + \sigma_0 \varepsilon'_{eff} (T^4 - T_w^4),$$

where α_{eff} , α'_{eff} – effective heat transfer coefficients ε_{eff} , ε'_{eff} – effective emissivities of surfaces, h_S and h_R – substrate and powder layer thicknesses; T_0 – temperature of the environment; T_w – temperature of the walls with which the heat is exchanged by radiation.

The second term $3K_{eff}\alpha_{T,eff}T\partial\varepsilon_{kk}/\partial t$ also contains effective properties (bulk elastic modulus K_{eff} and linear thermal expansion coefficient $\alpha_{T,eff}$). It reflects the coupling of heat transfer and deformation processes. Chemical reactions take place only in the powder. Then multiplier $h_R/(h_S + h_R)$ can be accounted for as corrections to the thermal effects of the reactions $Q'_k = h_R Q_k / (h_S + h_R)$. The external heat source can also be modified. For example, in the case of a laser it is

$$W'_{ext,eff} = \frac{W_{ext,eff}}{h_S + h_R} = \frac{(1 - f_L) W_0}{h_S + h_R k S_L} f(x, y) = q_0 f(x, y),$$

where S_L – effective heating spot area; W_0 – laser power; f_L – reflection coefficient; k – concentration factor (or correction factor); q_0 – effective power density of the heat source; type of function $f(x, y)$ depends on the mode and frequency of scanning. In this form (with the introduction of q_0 and $f(x, y)$), the source corresponds to any of the aforementioned movable heat sources. In the model (4) that takes into account the coupling of thermal and mechanical processes it is used not isobaric (or isochoric) heat capacity but heat capacity at constant strains c_ε .

2. Equilibrium problem

To determine deformations ε_{ij} one needs to solve the equilibrium problem of a planar object. For the plane stress state the following relations are true

$$\sigma_{zz} = 0, \quad \sigma_{xy} = \sigma_{xz} = \sigma_{yz} = 0, \quad (5)$$

$$\varepsilon = \begin{vmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ \varepsilon_{yx} & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_{zz} \end{vmatrix}. \quad (6)$$

Then there are two equations of equilibrium:

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0; \quad \frac{\partial \sigma_{yx}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} = 0. \quad (7)$$

Components of the strain tensor are related to components of the displacement vector by Cauchy relations

$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x}; \quad \varepsilon_{yy} = \frac{\partial u_y}{\partial y}; \quad \varepsilon_{xy} = \frac{1}{2} \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right), \quad (8)$$

where u_x, u_y – displacement vector components.

The additional relations are the equation

$$\frac{\partial^2 \varepsilon_{xx}}{\partial y^2} + \frac{\partial^2 \varepsilon_{yy}}{\partial x^2} = 2 \frac{\partial^2 \varepsilon_{xy}}{\partial x \partial y}. \quad (9)$$

and the Duhamel–Neumann relations

$$\sigma_{ij} = 2\mu_{eff}\varepsilon_{ij} + \delta_{ij} [\lambda_{eff}\varepsilon_{kk} - \langle K\omega \rangle], \quad (10)$$

where λ, μ – Lamet coefficients ($K = \lambda + 2\mu/3$), $i, j = x, y, z$; ω is a function of concentrations and temperature:

$$\omega = 3 \left[\alpha_T (T - T_0) + \sum_{k=0}^n \alpha_k (\eta_k - \eta_{k0}) \right], \quad (11)$$

α_k – concentration expansion coefficients; index "0" refers to the undeformed state; n – number of components; δ_{ij} – Kronecker delta: $\delta_{ij} = 1$, if $i = j$ and $\delta_{ij} = 0$, if $i \neq j$.

Designation $\langle K\omega \rangle$ means averaging over coating and

$$\begin{aligned} \langle K\omega \rangle &= \frac{1}{h_S + h_R} [K_S w_S h_S + K_R w_R h_R] = \\ &= \frac{K_S h_S \alpha_S + K_R h_R \alpha_R}{h_S + h_R} (T - T_0) + \frac{h_R K_R}{h_S + h_R} \sum_{k=0}^n \alpha_k (\eta_k - \eta_{k0}) = \\ &= K_{eff} \left[\alpha_{T,eff} (T - T_0) + \sum_{k=0}^n \alpha_{k,eff} (\eta_k - \eta_{k0}) \right] = K_{eff} \omega_{eff}. \end{aligned}$$

In what follows index «*eff*» and dash «'» in properties and effective parameters are omitted for simplicity.

Then for the plane stress state one can find from (10) that

$$\varepsilon_{xx} = \frac{\sigma_{xx}}{2\mu} - \left[\frac{\lambda}{2\mu} \frac{\sigma_{xx} + \sigma_{yy}}{3K} - \frac{\omega}{3} \right]; \quad \varepsilon_{yy} = \frac{\sigma_{yy}}{2\mu} - \left[\frac{\lambda}{2\mu} \frac{\sigma_{xx} + \sigma_{yy}}{3K} - \frac{\omega}{3} \right]; \quad (12)$$

$$\varepsilon_{zz} = - \left[\frac{\lambda}{2\mu} \frac{\sigma_{xx} + \sigma_{yy}}{3K} - \frac{\omega}{3} \right]; \quad \varepsilon_{xy} = \frac{\sigma_{xy}}{2\mu}. \quad (13)$$

The strain tensor and the stress tensor are symmetric, $\varepsilon_{xy} = \varepsilon_{yx}$.

After simple transformations [9] one can obtain from (2), (8) and (9) the system of equations

$$\Delta \sigma_{kk} = - \frac{K\mu}{\lambda + \mu} \Delta \omega, \quad \Delta \sigma_{yy} = \frac{\partial^2 \sigma_{kk}}{\partial x^2}, \quad \Delta \sigma_{xy} = - \frac{\partial^2 \sigma_{kk}}{\partial x \partial y}. \quad (14)$$

The remaining component of the stress tensor follows from the obvious relation $\sigma_{xx} = \sigma_{kk} - \sigma_{yy}$. Components of the strain tensor follow from (12)–(13).

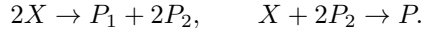
At the initial moment of time $t = 0$

$$\sigma_{ij} = 0; \quad \varepsilon_{ij} = 0. \quad (15)$$

Since the plate is free on the substrate, the stresses on all its surfaces are zero. However, any end fixation conditions can be set in the model.

3. Kinetics of composite formation

Suppose that a composite material is synthesized on a substrate from a mixture of powders in which the formation of strengthening particles occurs simultaneously with the formation of the matrix composition. It is assumed, as in [6, 9], that the process of composite synthesis can be described by two successive-parallel stages: one of the products of reaction P_2 , in which strengthening particles P_1 are formed, goes to the formation of matrix P according to some total reaction:



The presence of different components in the initial mixture X affects the rates of total stages. The rate of the first reaction is Φ_1 , second – Φ_2 .

Hereinafter concentrations of components for the written out total reaction scheme is denoted by the same letters as the symbols in this scheme. Then system of kinetic equations (2) has the following form

$$\frac{dP_1}{dt} = \Phi_1, \quad \frac{dP_2}{dt} = 2[\Phi_1 - \Phi_2], \quad \frac{dP}{dt} = \Phi_2. \quad (16)$$

The total reagent $X = 1 - P_1 - P_2 - P$.

It is assumed that reaction rates depend on concentrations according to the acting masses law and on temperature according to the Arrhenius law

$$\Phi_1(T) = k_{10}W_1(T)X^2; \quad \Phi_2(T)_2 = k_{20}W_2(T)P_2^2X,$$

$$W_1(T) = \exp\left(-\frac{E_{a1}}{RT}\right), \quad W_2(T) = \exp\left(-\frac{E_{a2}}{RT}\right),$$

where k_{10} and k_{20} are pre-exponential factors, E_{a1} and E_{a2} are activation energies of total reactions, R is the universal gas constant.

Consequently, the total chemical heat release in reactions is written as follows $W_{ch} = Q_1\Phi_1 + Q_2\Phi_2$, where Q_k are heat effects of reactions 1 and 2.

The rate of reactions involving solids can depend not only on temperature but also on stresses. A reaction can be activated not only by changing internal energy but also by mechanical work. Then [10]

$$W_1 = \exp\left[-\frac{E_{a1} - k_{\sigma 1}\Pi}{RT}\right], \quad W_2 = \exp\left[-\frac{E_{a2} - k_{\sigma 2}\Pi}{RT}\right], \quad (17)$$

where $k_{\sigma 1}, k_{\sigma 2}$ are coefficients of sensitivity of reaction rates to mechanical work (proportional to activation volumes); $\Pi = -(\sigma_{xx}\varepsilon_{xx} + \sigma_{yy}\varepsilon_{yy} + 2\sigma_{xy}\varepsilon_{xy})$ – mechanical work.

As a result, the heat conduction equation takes the form

$$c_\varepsilon\rho\frac{\partial T}{\partial t} = \lambda_T\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + Q_1\Phi_1 + Q_2\Phi_2 - H + W_{ext} - 3K\alpha_T T\frac{\partial \varepsilon_{kk}}{\partial t}. \quad (18)$$

Next, let us assume that $W_{ext} = q_0 \exp(-((x - Vt)^2 + y^2)/a_t^2)$, $H = \alpha_{eff}(T - T_0) + \sigma_0\varepsilon_0(T^4 - T_w^4)$.

Thus, the thermokinetic problem involves kinetic equations (16) and heat conduction equation (18). Conditions for this part of the problem are

$$t = 0 : T = T_0, \quad X = 1, \quad P = P_1 = P_2 = 0;$$

$$y = 0 : \quad \partial T/\partial y = 0, \quad x = 0, \infty : \quad \partial T/\partial x = 0, \quad y \rightarrow \infty : \quad \partial T/\partial y = 0.$$

4. Problem in dimensionless form

The nature of processes occurring in the plate depends on the ratio of different physical scales which in turn depend on the properties characterizing different physical processes. Properties in the process of reactions continuously change, and it is impossible to find data to describe the change of properties so effective properties were introduced above. Further, in order to study phenomena qualitatively, it is advisable to switch to dimensionless variables. They significantly reduce the number of unknown quantities and allow us to develop a convenient algorithm for the numerical realization of the model.

Let us introduce dimensionless variables

$$\theta = \frac{T - T_*}{T_* - T_0}, \quad \tau = \frac{t}{t_*}, \quad \xi = \frac{x}{x_*}, \quad \eta = \frac{y}{x_*}, \quad e_{ij} = \frac{\varepsilon_{ij}}{\varepsilon_*}, \quad s_{ij} = \frac{\sigma_{ij}}{\sigma_*}, \quad \bar{\Pi} = \frac{\Pi}{\varepsilon_* \sigma_*},$$

where

$$T_* = \frac{Q_1}{c\rho} + T_0, \quad t_* = \frac{c\rho RT_*^2}{k_{01} E_{a1} Q_1} \exp\left(\frac{E_{a1}}{RT_*}\right), \quad x_* = \sqrt{\frac{\lambda t_*}{c\rho}},$$

$$\sigma_* = 3K\alpha_T(T_* - T_0), \quad \varepsilon_* = \frac{3K\alpha_T(T_* - T_0)}{2\mu}.$$

As a result, the problem takes the form similar to [9]

$$\frac{\partial \theta}{\partial \tau} = \left[\frac{\partial^2 \theta}{\partial \xi^2} + \frac{\partial^2 \theta}{\partial \eta^2} \right] + \frac{1}{\theta_0} \bar{\Phi}_1 + S_{ch} z_{ch} \frac{1}{\theta_0} \bar{\Phi}_2 + f_1 - S_b \left[(\theta + \sigma^{-1})^4 - (\sigma^{-1} - \theta_w)^4 \right] -$$

$$- Bi(\theta + 1) - (\theta + \sigma^{-1}) \kappa^{-1} \delta_\varepsilon \frac{\partial e_{kk}}{\partial \tau} \quad (19)$$

$$\frac{dP}{d\tau} = \gamma \bar{\Phi}_1; \quad \frac{dP_1}{d\tau} = 2\gamma(\bar{\Phi}_1 - \bar{\Phi}_2); \quad \frac{dP_2}{d\tau} = \gamma \bar{\Phi}_2, \quad (20)$$

$$\Delta s_{kk} = -\frac{\kappa}{2 - \kappa} \Delta \bar{w}; \quad \Delta s_{\eta\eta} = \frac{\partial^2 s_{kk}}{\partial \xi^2}; \quad \Delta s_{\xi\eta} = \frac{\partial^2 s_{kk}}{\partial \xi \partial \eta}; \quad s_{\xi\xi} = s_{kk} - s_{\eta\eta}. \quad (21)$$

At the initial moment of time

$$\tau = 0 \quad \theta = -1; \quad X = 1, \quad P_1 = 0, \quad P_2 = 0, \quad s_{ij} = 0 \quad (22)$$

Boundary conditions for the thermokinetic problem are

$$\xi \rightarrow 0, L_\xi : \quad \frac{\partial \theta}{\partial \xi} = 0; \quad \eta \rightarrow 0, L_\eta : \quad \frac{\partial \theta}{\partial \eta} = 0; \quad (23)$$

and for the equilibrium problem are

$$\xi = 0, \quad \xi = L_\xi : \quad s_{ij} = 0; \quad \eta = 0, \quad \eta = L_\eta : \quad s_{ij} = 0. \quad (24)$$

It is assumed in (19), (20) that

$$f_1 = S_e \exp\left(-\frac{(\xi - \bar{V}\tau)^2 + \eta^2}{\delta_t^2}\right);$$

$$\bar{\Phi}_1 = X^2 \exp\left[\frac{\theta\sigma - \delta_\varepsilon A_1 \bar{\Pi}}{\beta(1 + \theta\sigma)}\right]; \quad \bar{\Phi}_2 = P_2^2 X \exp\left[\frac{\theta\sigma + e_k - \delta_\varepsilon A_2 \bar{\Pi}}{\beta(1 + \theta\sigma)}\right].$$

$$e_{kk} = e_{\xi\xi} + e_{\eta\eta} + e_{\zeta\zeta}; \quad \bar{\Pi} = -(e_{\xi\xi} s_{\xi\xi} + e_{\eta\eta} s_{\eta\eta} + 2e_{\xi\eta} s_{\xi\eta})$$

$$\bar{w} = [(\theta + 1) + g_1 (P_1 - P_{10}) + g_2 (P_2 - P_{20}) + g_0 (P - P_0)].$$

The remaining values are also reduced to dimensionless form.

In general, solution of the problem depends on a large number of parameters. Their definition in terms of physical scales and the ranges of change is given in Tab. 1. All parameters of the problem have a clear physical meaning and they are described in [6, 9]. The algorithm of numerical solution of the problem is described there and the role of chemical reactions in the total values of stresses and strains is demonstrated. However, some important aspects of the problem formulation are not reflected there.

Ranges of variation of dimensionless parameters were determined using literature data on the properties of various substances (*Ti*, *Al*, *Cr*, *Fe* oxides) and parameters of heat sources and kinetic constants (q_0 , V , E_{ai} , Q_i , k_{0i}) [9].

Table 1. Parameters of the model and their ranges of variation.

Dimensionless parameter	Range of variation of dimensionless parameter	Dimensionless parameter	Range of variation of dimensionless parameter
$\gamma = \frac{(cp)_S RT_*^2}{E_{a1} Q_1}$	$\gamma = 0.009 \div 0.1$	$S_{ch} = \frac{Q_2}{Q_1}$	$S_{ch} = 0.1 \div 1$
$\sigma = \frac{T_* - T_0}{T_*}$	$\sigma = 0.3 \div 0.9$	$z_{ch} = \frac{k_2}{k_1}$	$z_{ch} = 10^{-6} \div 10^6$
$\theta_0 = \frac{\sigma}{\beta}$, $\beta = \frac{E_{a1}}{RT_*}$	$\theta_0 = 4 \div 15$	$e_k = 1 - \frac{E_{a2}}{E_{a1}}$	$e_k = 0 \div 0.7$
$S_b = \frac{t_* \sigma_0 \varepsilon_0 (T_* - T_0)^3}{c_S \rho_S}$	$S_b = 10^{-6} \div 10^{-4}$	$S_e = \frac{q_0}{h} \frac{t_*}{(T_* - T_0) c_S \rho_S}$	$S_e = 10^{-8} \div 10^3$
$Bi = \alpha_{eff} \frac{t_*}{c_S \rho_S}$	$Bi = 0 \div 4$	$\delta_\varepsilon = \frac{(3K\alpha_T)^2 (T_* - T_0)}{2\mu cp}$	$\delta_\varepsilon = 0 \div 0.1$
$\theta_w = \frac{T_* - T_w}{T_* - T_0}$	$\theta_w = 0.4 \div 0.9$	$\delta_t = a_t / x_*$	$\delta_t = 0.03 \div 10^5$
$g_i = \frac{(\alpha_i - \alpha_x)}{\alpha_T (T_* - T_0)}$	$g_i = -4 \div 4$	$\bar{V} = V t_* / x_*$	$\bar{V} = 10^{-8} \div 10^3$
$A_1 = \frac{k_{\sigma 1} Q_1}{E_{a1}}$ $A_2 = \frac{k_{\sigma 2} Q_1}{E_{a1}}$	$A = 0 \div 20$	–	–

5. Analysis of results

In the course of calculations, parameters were varied within a fairly wide range. In the examples presented below, some of the parameters were fixed [9]: $z_{ch} = 100$, $e_k = -0.2$, $A = 0.4$, $g_0 = 3.72$, $g_1 = -0.62$, $g_2 = 3.24$; $\bar{V} = 0.25$, $S_e = 2.5$, $K_C = 1$; $S_{ch} = 0.5$, $\delta_t = 2$, $\sigma = 0.5$, $\beta = 0.025$, $\gamma = 0.035$, $S_b = 0.0015$,

The synthesis control conditions are fixed. To illustrate the interrelation of processes of different nature let us limit ourselves to a single pass. For chosen control parameters for a single pass after the unsteady stage the process changes to a stationary regime in which the temperature values, the shape of temperature distributions and the accompanying stress and strain distributions remain practically unchanged. However, this cannot be stated for multi-pass processing. The dynamics of the process for different situations is shown in [6–9] and it is not duplicated here. The composition of the composite behind the laser beam, i.e., where the external source is absent, no longer changes. This "quasi-stationary" composition depends both on parameters characterizing the processing conditions and on the interaction of different physical processes.

This is illustrated in Fig. 1. The higher parameter Bi the greater heat loss, the lower temperature and, obviously, the lower yield of the reaction product (Fig. 1,a). The higher sensitivity coefficients to mechanical work the faster reactions start and the higher yield of products.

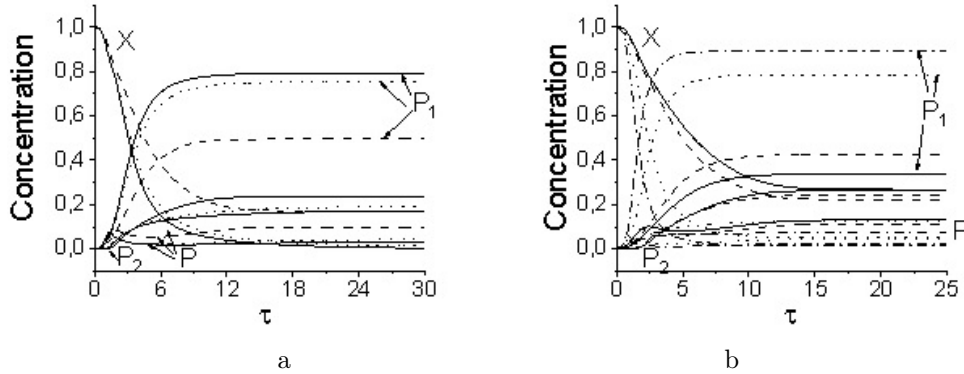


Fig. 1. Time dependence of composition at the point ($x=25, y=0$) for various conditions of heat exchange with the environment (a) and for various relationships between reaction rate and mechanical work (b). Parameters are $\delta_\varepsilon = 0.05, g_k \neq 0$. In figure (a) $\delta_k = 0.05$, solid lines — $Bi = 0$; dashed lines — $Bi = 0.1$; dotted-lines — $Bi = 0.5$. In figure (b) $\delta_\varepsilon = 0.05$; solid lines — $\delta_k = 0$; dashed lines — $\delta_k = 0.05$; dotted-lines — $\delta_k = 0.25$; dashed-dotted-lines — $\delta_k = 0.5$

The values of stresses and strains also depend significantly on the model parameters (Figs. 2–4). With increasing heat losses (curves 1–3) in Fig. 2, a,b stresses and strains decrease due to decreasing temperature, decreasing size of the region where gradients are significant, and slowing down of chemical reactions. The maximum corresponds to the coordinate of the heat source position at a given time. The behaviour of diagonal components of tensors is qualitatively similar to that of invariants s_{kk} and e_{kk} . The shear stresses and strains at the chosen set of parameters are much smaller and their behaviour is different from that of diagonal components (Fig. 2,c,d).

The shape of curves shown in Fig. 2,a, b corresponds to the qualitative temperature distribution (Fig. 3). For $Bi = 0$ (curves 1) the sample warms up in front of the beam due to heat conduction and initiated chemical reactions, and since there are no heat losses from the end the heat is accumulated. Although there are edge effects associated with overheating in experimental studies, $Bi = 0$ hardly corresponds to laser treatment. For $Bi = 0.1$ (curves 2) temperature is much lower but heat conduction still favours heating in front of the heat source which promotes preheating. For $Bi = 0.5$ (curves 3) a temperature profile typical for quasi-stationary laser treatment is observed.

Fig. 4 illustrates the role of concentration stresses and strains which can be comparable to thermal stresses in absolute value [9]. For selected values of parameters the consideration of concentration stresses leads to an increase in the total value of stresses and strains. Shear stresses and strains are highlighted in Fig. 4 c,d

As noted above, there are two types of coupling in the heat conduction equation. It is found that neglecting one of them also changes the result. Thus, if there is no coupling in the traditional sense (Fig. 5, left, $\tau = 30$) but the coefficient of sensitivity of reaction rates to mechanical work is not equal to zero the distributions of all physical quantities along the coordinate are qualitatively and quantitatively different from those when coupling is fully taken into account (Fig. 5, right,

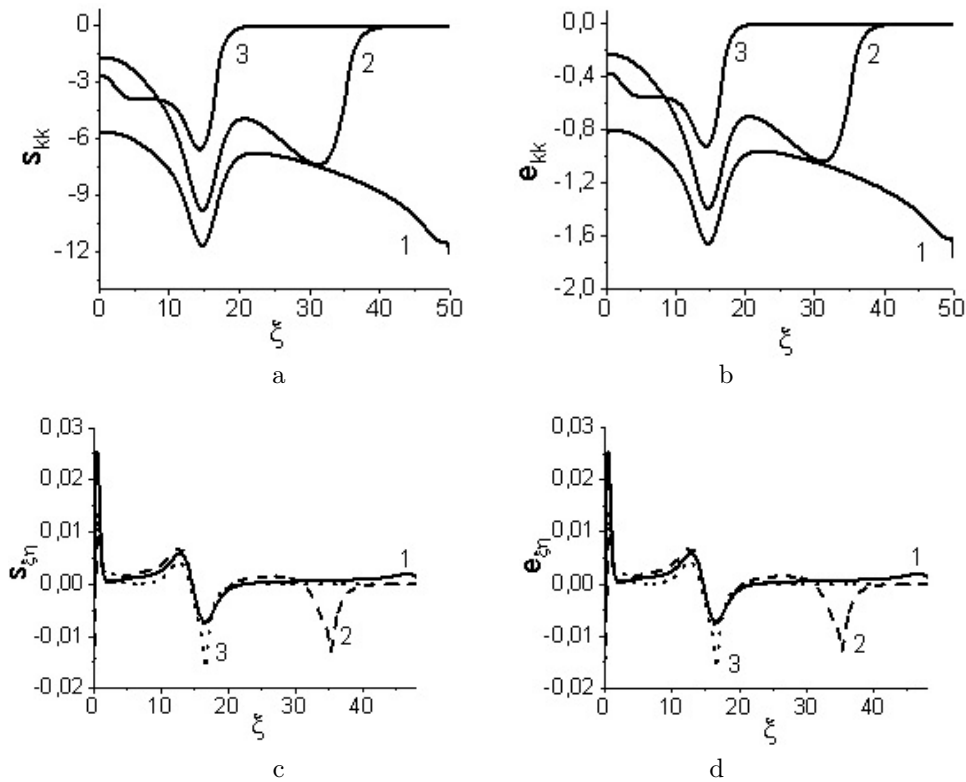


Fig. 2. Distributions along the axis of laser motion at time $\tau=60$ of the first invariants of stress (a) and strain (b) tensors and shear components (c) and (d) of tensors. Parameters are $\delta_\varepsilon = 0.05$, $\delta_k = 0.05$; $g_k \neq 0$; 1 – $Bi = 0$; 2 – $Bi = 0.1$; 3 – $Bi = 0.5$

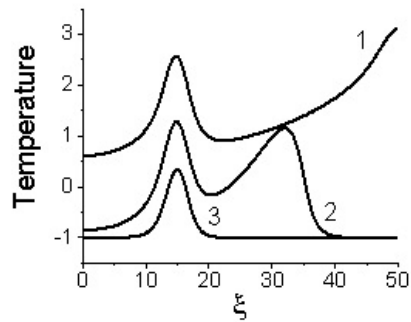


Fig. 3. Temperature distribution at $\tau = 40$ for various conditions of heat exchange with the environment 1 – $Bi = 0$; 2 – $Bi = 0.1$; 3 – $Bi = 0.5$. $\delta_\varepsilon = 0.05$, $\delta_k = 0.05$; $g_k \neq 0$

$\tau = 60$). The second maximum in stresses and strains is associated with the acceleration of reactions in front of the moving heat source due to mechanical work. Note that composition for these variants is also different (not shown in the figures). More interesting results are obtained in coupled models when reverse stages of chemical reactions are taken into account.

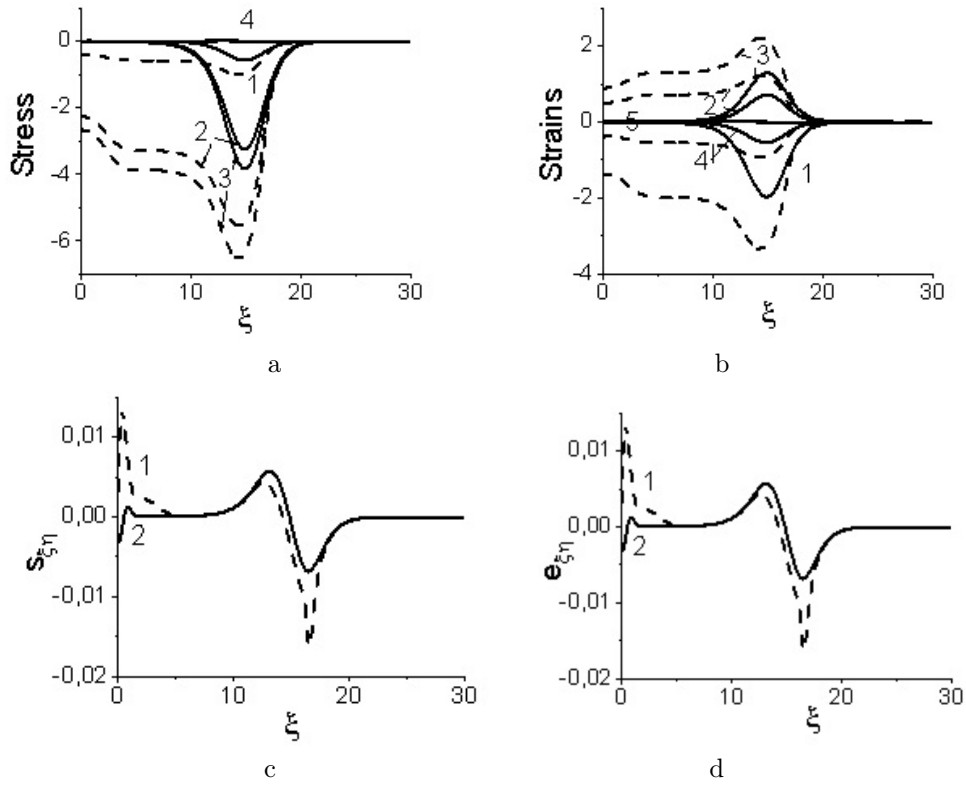


Fig. 4. Distributions along the axis of laser motion at time $\tau=60$ of the first invariants of stress (a) and strain (b) tensors and shear components (c) and (d) of tensors. Parameters are $\delta_\varepsilon = 0.05$, $\delta_k = 0.05$. In figure (a): 1 – $s_{\xi\xi}$, 2 – $s_{\eta\eta}$, 3 – s_{kk} , 4 – $s_{\xi\eta}$. In figure (b): 1 – $e_{\xi\xi}$, 2 – $e_{\eta\eta}$, 3 – $e_{\xi\xi}$, 4 – e_{kk} , 5 – $e_{\xi\eta}$. Solid lines – $g_i = 0$; dotted lines – $g_i \neq 0$

Conclusion

The paper describes a model of controlled synthesis on a substrate. It is shown that the model has several channels of interaction between different physical phenomena accompanying the synthesis. Even if it is assumed that properties do not depend on composition and temperature it is possible to identify features of coupled models useful for process control in real conditions. For example, acceleration of reactions in front of a heat source. Note that such an approach to study dynamics of synthesis of new materials can be useful for various variants of combined technologies [11–13].

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Влияние связанности термокинетических и механических процессов на синтез композита на подложке

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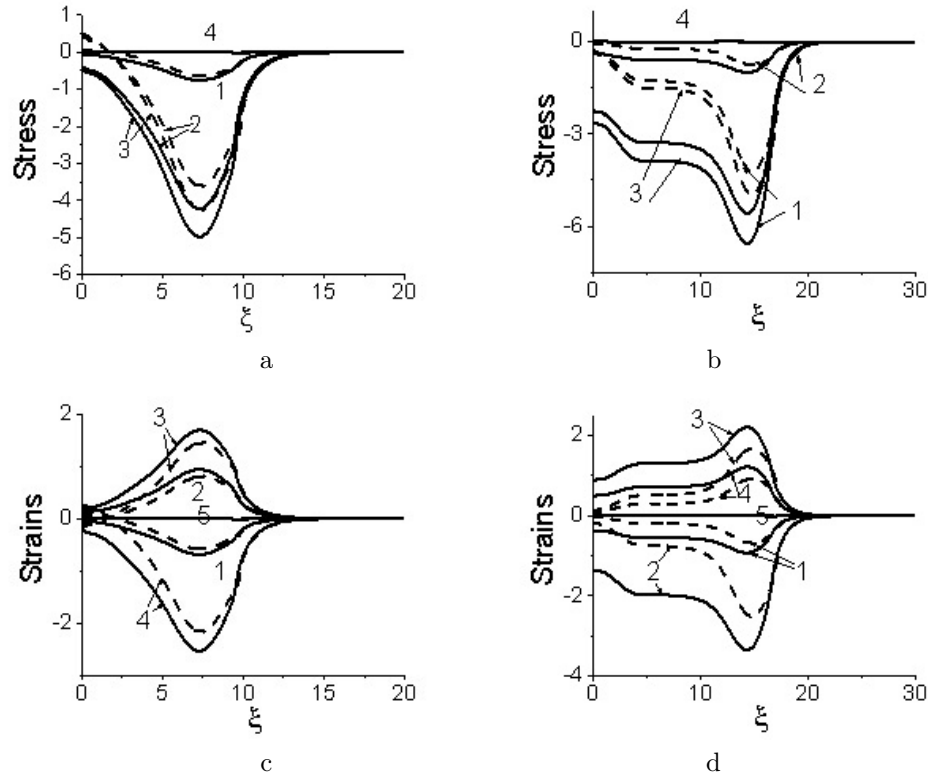


Fig. 5. Distributions along the axis of laser motion of the first invariants of stress (a, b) and strain (c, d) tensors. In figures (a, b) 1 — $s_{\xi\xi}$, 2 — $s_{\eta\eta}$, 3 — s_{kk} , 4 — $s_{\xi\eta}$; $\delta_\epsilon = 0$, solid line — $\delta_k = 0.25$, dotted line — $\delta_k = 0.5$. In figures (c, d): 1 — $e_{\xi\xi}$, 2 — $e_{\eta\eta}$, 3 — $e_{\zeta\zeta}$, 4 — e_{kk} , 5 — $e_{\xi\eta}$; $\delta_\epsilon = 0.05$. Solid lines — $\delta_k = 0.05$, dotted lines — $\delta_k = 0.25$

Аннотация. Представлена связанная математическая модель процесса синтеза композита из порошковой смеси в условиях лазерного нагрева. Модель учитывает два явления, которыми пренебрегают в традиционных моделях обработки поверхности и 3D-технологий: взаимное влияние теплопереноса и деформации и выделение тепла в химических реакциях. Формирование состава описывается упрощенной схемой реакций, включающей суммарную реакцию, приводящую к образованию упрочняющих частиц, и суммарную реакцию формирования матрицы. Учтено влияние работы напряжения на скорость реакции. Напряженно-деформированное состояние описывается в квазистатическом приближении. В результате показано, что связанность процессов различной физической природы важна как для определения состава композита, так и для оценки сопутствующих синтезу напряжений и деформаций.

Ключевые слова: связанная модель, синтез композитов, сопутствующие напряжения, контролируемый режим.