Thermo-visco-elastic model of powder layer modification by moving heat source

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Abstract. The coupled model for laser treatment of plate is presented in this paper. The model takes into account viscoelastic stresses and strains due to temperature and composition change. Heat capacity and viscosity depend on liquid phase fraction. The numerical algorithm is described. Examples demonstrate qualitative features appearing in the model with melting and heat losses into environment. The coupled and non-coupled models give different results.
Keywords: laser treatment, melting, viscoelastic stresses.

1. Introduction

There are fundamentally different methods of synthesizing 3D material in powder technology. In one of them, the powder is preliminary sprayed on the surface to be treated and then the surface is scanned by laser radiation or an electron beam. In the other, the powder is fed directly into a melt bath, which is pre-formed in the area of a moving energy source. In either case, the powder undergoes a change from a solid state to a liquid state and back; the entire process is accompanied by a variety of physical and chemical phenomena. Before the planetary scale boom in additive technologies, similar methods were actively developed for coating and surface treatment of materials. In mathematical modeling of the accompanying phenomena, the problem arises of selecting or constructing a suitable model that adequately describes the behavior of the material in both the solid and liquid phases, as well as in the two-phase region. Related to this is the variety of modeling approaches. Numerous publications analyze purely thermophysical models for calculating temperature fields at different variants of the heat source setting; study the behavior of fine particles in the melt bath; describe powder melting and melt flow in the unmelted powder, including using filtration theory; analyze variants for calculating residual stresses, etc.

In spite of the fact that each of the approaches allows obtaining interesting results and studying a number of phenomena, the process of creating a new material in dynamics and accompanying phenomena prove to be insufficiently studied.

The present work aims to formulate the coupled model the treatment by moving heat source of powder layer placed on a substrate assuming that material conversion «powder-liquid-solid» cab be characterized by changing viscoelastic properties.

2. General equations

A Maxwell-type model is used as the basis, which allows a transition to both a fluid and an elastic body when the shear viscosity coefficient changes [1]. Within the framework of this model, the relations

$$\frac{d\sigma_{ij}}{dt} + \frac{\mu}{\kappa}\sigma_{ij} = 2\mu\frac{d\varepsilon_{ij}}{dt} + \delta_{ij}\left[\frac{d}{dt}(\lambda\varepsilon_{kk} - K\omega) + \frac{\mu}{\kappa}K(\varepsilon_{kk} - \omega)\right]. \tag{1}$$

Here κ is shear viscosity coefficient; $K = \lambda + 2\mu/3$ is bulk module; λ, μ are Lamé coefficients; the function ω depends on temperature and composition

$$\omega = 3\left[\alpha_T(T - T_0) + \sum_{k=1}^{n}\alpha_k(C_k - C_{k,0})\right], \tag{2}$$

where α_T is the thermal expansion coefficient; C_k are species concentrations; α_k are the coefficients of concentration expansion; index «0» relates to an initial state.

In limiting case $\kappa \to \infty$ we come from (1) to

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \delta_{ij}\left[\lambda\varepsilon_{kk} - K\omega\right] \tag{3}$$

In the case of $\kappa \to 0$, we have the relation between stress σ_{ij} and strain ε_{ij} components similar ideal fluid with spherical stress tensor.

In the literature, such models are used to describe the mechanical behavior of media with both liquid and solid properties. Viscous and/or elastic-viscous-plastic properties often characterize materials undergoing structural transformations [2], solid materials with diffusion-controlled chemical reactions [3]; composites [4], materials used in pharmaceuticals [5]. Powder media behave similarly to a viscous liquid [6]. In [7] an attempt has been made to describe the change in the thickness of a thin powder layer due to the change in porosity during the electron beam treatment on the basis of model (1).

In the present paper, we use the Maxwell model (1), taking into account changes in the heat capacity and viscosity around the melting point, to build a more detailed model of the surface treatment of the material by laser radiation. In our case, this is quite a suitable model, since the reactants and reaction products can be in both solid and liquid states; there are regions with different rheological properties in the treatment zone. To the equations written out we should add the energy equation in the form of the heat conduction equation, as well as the kinetics equations describing the change in composition.

For a specimen that has the shape of a thin plate or layer located on a flat substrate, we accept the following assumptions: (1) the specimen is in a plane stress state; in this case, $\sigma_{zz} = \sigma_{xz} = \sigma_{yz} = 0$; (2) chemical reactions can take place in the treated layer, which we describe by the summarized "reagent-product" scheme; (3) material is considered incompressible. Then we assume that of all properties, only heat capacity and viscosity depend significantly on temperature.

It is known that in the vicinity of the melting point the heat capacity increases sharply, which in classical theory is described by the Dirac delta function. For simple or single-component materials, this is quite a suitable way to describe it. However, for binary systems (e.g., two kinds of powders), the appearance of a two-phase zone – a region where liquid (fusible component) and solid phase (refractory particles) are simultaneously present – begins to play an important role in the melting process. In this case, to describe the melting process, we can introduce two temperatures T_1 and T_2. The first will correspond to the melting temperature of the fusible component, the second to the melting temperature of the refractory particles. Between these two temperatures, the fraction of liquid phase η_L in the system will change from 0 to 1 according to some law $\eta_L = \eta_L(T)$.

The viscosity for the powder medium, the melt with particles, the fully melted particle mixture and the final material after solidification can vary considerably. For simplicity, we will assume that the viscosity depends on the fraction of the liquid phase and changes from the effective viscosity of the powder medium, to the viscosity of the melt, and then on cooling (away from heat sources) to the viscosity of the new material. There are no experimentally established or theoretically substantiated laws in the literature for κ when phase and chemical composition change. Therefore, we use the simplest linear approximation in the model. For example, in the case of melting, $\kappa = \kappa_p (1 - \eta_L) + \kappa_L\eta_L$.

Next, assume that the chemical reactions leading to the formation of the product begin when the liquid phase appears. Then the kinetic equation describing the process as a whole will look like

$$\frac{d\eta}{dt} = k_0\phi(\eta)\eta_L \exp\left(-\frac{E_A \pm \alpha_V\Pi}{RT}\right) = \Phi(\eta,\eta_L,T,\Pi),$$

where k_0 is an pre-exponential factor; E_A is activation energy of the total chemical reaction; α_V is the sensitivity coefficient of the reaction rate to the work of mechanical stresses Π; $\varphi(\eta)$ is some kinetic function; R is universal constant gas.

To simplify the situation, let's assume that the laser beam is expanded in a line, which leads to an effective heat source of the form:

$$W_{ext} = q_0 \exp\left(-\left(\frac{x - Vt}{a}\right)^2\right),$$

where a is an effective source radius; V is its velocity along the surface.

I.e. now we have all quantities independent of z or y:

$$\sigma_{xy} = 0; \varepsilon_{xy} = 0; \varepsilon_{yy} = 0; \varepsilon_{kk} \approx \varepsilon_{xx} + \varepsilon_{zz}$$

As a result, the model will include one-dimensional, but coupled equations:

$$c_\varepsilon \rho \frac{\partial T}{\partial t} = \lambda_T \frac{\partial^2 T}{\partial x^2} + W_{ch} + W_{ext} + D - \alpha_{eff}(T - T_0) - 3K\alpha_T T\left(\frac{\partial \varepsilon_{xx}}{\partial t} + \frac{\partial \varepsilon_{zz}}{\partial t}\right);$$

$$\frac{\partial^2 \sigma_{xx}}{\partial x^2} = \rho \frac{\partial^2 \varepsilon_{xx}}{\partial t^2};$$

$$\frac{\partial \sigma_{xx}}{\partial t} + \frac{\mu}{\kappa}\sigma_{xx} = 2\mu\frac{\partial \varepsilon_{xx}}{\partial t} + \left[\frac{\partial}{\partial t}(\lambda\varepsilon_{kk} - K\omega) + \frac{\mu}{\kappa}K(\varepsilon_{kk} - \omega)\right];$$

$$\frac{\partial \sigma_{yy}}{\partial t} + \frac{\mu}{\kappa}\sigma_{yy} = \frac{\partial}{\partial t}(\lambda\varepsilon_{kk} - K\omega) + \frac{\mu}{\kappa}K(\varepsilon_{kk} - \omega);$$

$$0 = 2\mu\frac{\partial \varepsilon_{zz}}{\partial t} + \left[\frac{\partial}{\partial t}(\lambda\varepsilon_{kk} - K\omega) + \frac{\mu}{\kappa}K(\varepsilon_{kk} - \omega)\right]; \quad \frac{d\eta}{dt} = \Phi(\eta, \eta_L, T, \Pi),$$

where α_{eff} is some effective coefficient of heat loss to the environment by convection and to the substrate; $W_{ch} = Q(d\eta/dt)$ is the heat source associated with chemical reactions; $D = \sigma_{xx}(\partial \varepsilon_{xx}/\partial t)$ is the viscous dissipation.

Thus, for the six variables T, η, σ_{xx}, ε_{xx}; σ_{yy}, ε_{zz} we have six equations.

At the initial moment of time $t = 0$ we have

$$T = T_0; \eta = 0; \eta_L = 0; \sigma_{ij} = 0; \varepsilon_{ij} = 0.$$

3. Algorithm and Examples

The next step is to develop a computational algorithm. The main steps are as follows. (1) First, a transition to dimensionless variables is made; scale relations give dimensionless complexes, whose values determine the subsequent development of the algorithm. (2) The equations are then given a form that allows the use of known methods. Since the model is coupled and the equations cannot be completely separated, the numerical implementation of the model uses separation by physical processes; convergence is investigated by varying the spatial and time steps, and iterations at each time step may be applied. (3) Then, a detailed parametric study is carried out, which makes it possible to identify the peculiarities of the synthesis process in different regions of variation of the parameters responsible for the external control and the parameters reflecting the properties of

materials and the nature of their variation. The problem in the choice of the algorithm is also related to the presence of different stages – essentially nonstationary and almost stationary stage with a moving two-phase zone of constant size, where different coordinate and time step ratios turn out to be optimal from the viewpoint of minimizing the computational error.

The scales in the model are defined as follows

$$x_*^2 = \frac{\lambda_T t_*}{[c_\varepsilon \rho]_s} \; ; \; t_* = \frac{[c_\varepsilon \rho]_s RT_*^2}{EQk_0} \exp\left(\frac{E_a}{RT_*}\right) \; ; \; T_* = T_0 + \frac{Q}{[c_\varepsilon \rho]_s} \; ; \; \varepsilon_* = 3\alpha_T (T_* - T_0) \; ; \; \sigma_* = K\varepsilon_* .$$

The following dimensionless variables are used:

$$\theta = \frac{T - T_0}{T_* - T_0} \; ; \; \tau = \frac{t}{t_*} \; ; \; \xi = \frac{x}{x_*} \; ; \; S_i = \frac{\sigma_{ij}}{\sigma_*} \; ; \; e_i = \frac{\varepsilon_{ij}}{\varepsilon_*} .$$

Examples are presented below to illustrate the role of viscosity changes in the region where the liquid phase appears in the evolution of properties and associated stresses. There is no chemical reaction or it has no effect on either the properties or the temperature and stress fields. In the calculations, it is assumed that:

$$\sigma = \frac{T_0}{T_* - T_0} = 0.5 \; ; \; \gamma_1 = \frac{\lambda}{K} = 0.9 \; ; \; \Delta = \frac{\rho x_*}{t_*^2 K} = 0.3 \; ; \; \beta = \frac{\gamma}{1 + \sigma} \; ; \; \gamma = \frac{[c_\varepsilon \rho]_s RT_*^2}{EQk_0} = 0.1 \; ;$$

$$\theta_1 = \frac{T_1 - T_0}{T_* - T_0} = 0.7 \; ; \; \theta_2 = \frac{T_2 - T_0}{T_* - T_0} = 0.9 \; ; \; H = \frac{Q_m}{mQ} = 0.3 \; ; \; \tau_0 = \frac{\kappa_0}{\mu t_*} = 0.1 \; ; \; \tau_L = \frac{\kappa_L}{\mu t_*} = 0.05 \; ;$$

$$\overline{V} = \frac{Vt_*}{x_*} = 100 \; ; \; a = \frac{R_0}{x_*} = 0.0005 \; ; \; q = \frac{[c_\varepsilon \rho]_s W}{\pi Q} \frac{1}{\lambda_T} = 1.2 .$$

The heat source starts moving from the point $\xi = 0.1$. Sample length is $L = 10$.

Variant 1. If the problem is uncoupled, $\omega = 0$, there is no melting and no heat loss by convection, $Nu = 0$, where

$$\omega = 3\alpha_T (T_* - T_0) \frac{3K\alpha_T}{[c_\varepsilon \rho]_s} \; ; \; Nu = \alpha_{eff} \frac{t_*}{c_\varepsilon \rho} ,$$

then at this set of parameters at the initial stage the stresses in the direction of motion of the heat source practically repeat the change in temperature. Coming to a quasi-stationary regime corresponds to a practically unchanged temperature, in this case greater than 0.93; the size of the region with the maximum temperature and maximum stresses expands. Deformations e_z behave similarly (this is not shown in the drawings). In the steady-state stage, there is no complete similarity between all quantities. However, high stress and strain gradients take place where there are high temperature gradients, i.e., in the vicinity of the external heat source. The numerical values of all quantities depend on viscosity, which is unchanged in this case.

Variant 2. Taking melting into account, we get a generally similar picture, but both the maximum temperature (below 0.9, Fig.1a) and the maximum stresses decrease. At a given value $q = 1.2$, complete melting is not observed. There are two phases in the region left by the external source. The two-phase zone, bounded in Fig.1b by curves, gradually expands. In the same area, the heat capacity and viscosity change in a similar way.

Variant 3. Heat loss to the environment leads to a qualitative change: in the two-phase zone the temperature is not constant, the share of the liquid phase also changes gradually (Fig.2). Similar evolution is typical for other values. At the steady-state stage there appears a two-phase region of

constant size (Fig.3a, dotted curves), bounded, on the one hand, by the value of $\eta_L = 0$, and on the other hand, by the value of $\eta_{L,max}$, attainable at given parameters. The smaller is the value of $\eta_{L,max}$, the less changes in heat capacity and viscosity are evident.
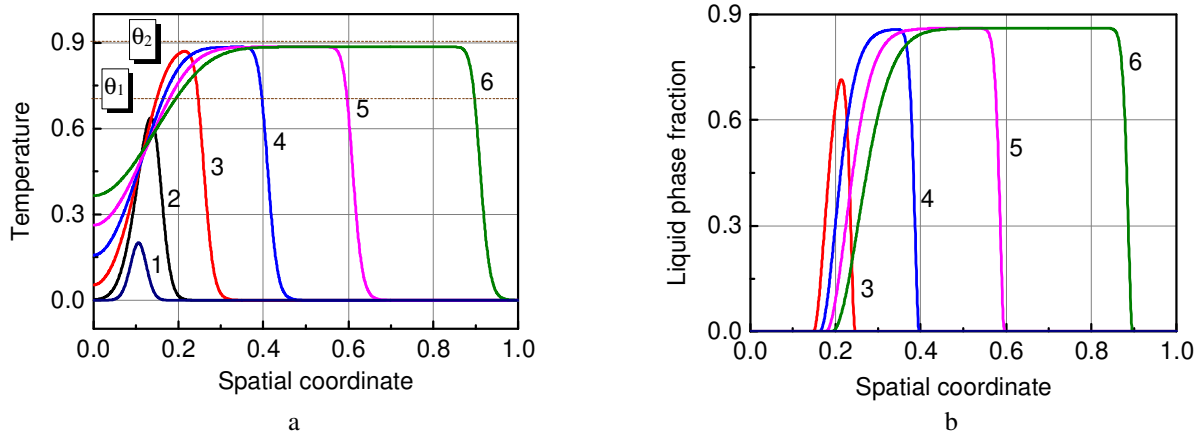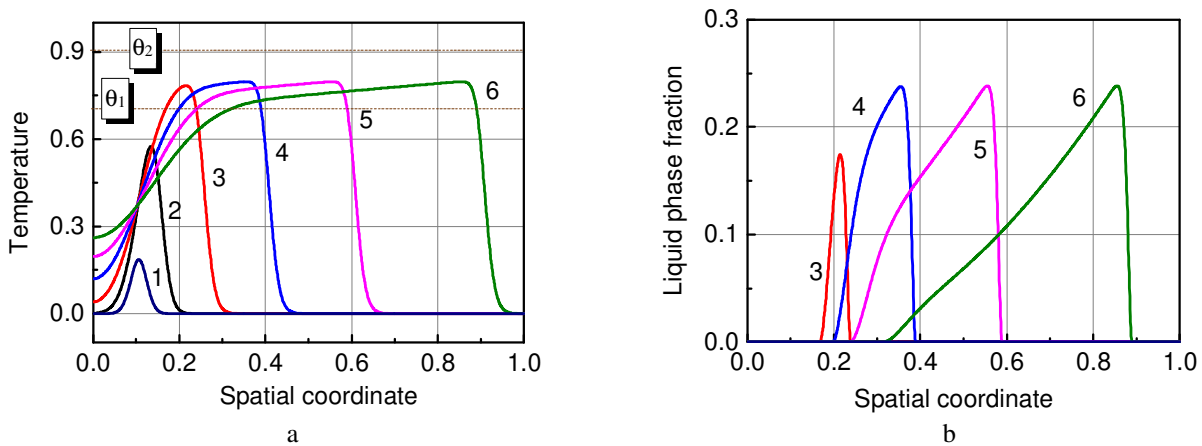

Fig.1. Temperature (a) and liquid phase fraction (b) distributions for variant 2. Time moments, τ: $1 - 10^{-4}$; $2 - 5 \cdot 10^{-4}$; $3 - 1.5 \cdot 10^{-3}$; $4 - 3 \cdot 10^{-3}$; $5 - 5 \cdot 10^{-3}$; $6 - 8 \cdot 10^{-3}$.

Fig.2. Temperature (a) and liquid phase fraction (b) distributions for variant 3. Time moments, τ: $1 - 10^{-4}$; $2 - 5 \cdot 10^{-4}$; $3 - 1.5 \cdot 10^{-3}$; $4 - 3 \cdot 10^{-3}$; $5 - 5 \cdot 10^{-3}$; $6 - 8 \cdot 10^{-3}$.

Variant 4. Let's compare temperature and liquid phase fraction distributions at steady-state stage (Fig.3a, Fig.3b) for uncoupled (dotted curves) and coupled ($\omega = 0.2$) models (solid curves in Fig.3a, Fig.3b). A small change in the maximum temperature leads to a significant decrease in the liquid phase fraction. The stresses (Fig.3c) are shown only for the time moment corresponding to curves 5. The energy distribution in the external source (Fig.3c) is also given for one time moment.

4. Conclusion

Thus, the paper presents a model of surface treatment by laser radiation, taking into account melting, possible chemical reaction and viscosity change with the appearance of the liquid phase fraction. The coupled nature of the model is manifested both in the accounting of viscous dissipation and in the possible change in the reaction rate. It is shown that accounting for heat losses to the environment leads to a qualitative change in temperature and property distributions. The appearance of a two-phase zone of constant dimensions at the steady-state stage is due to the interaction of processes of different nature.
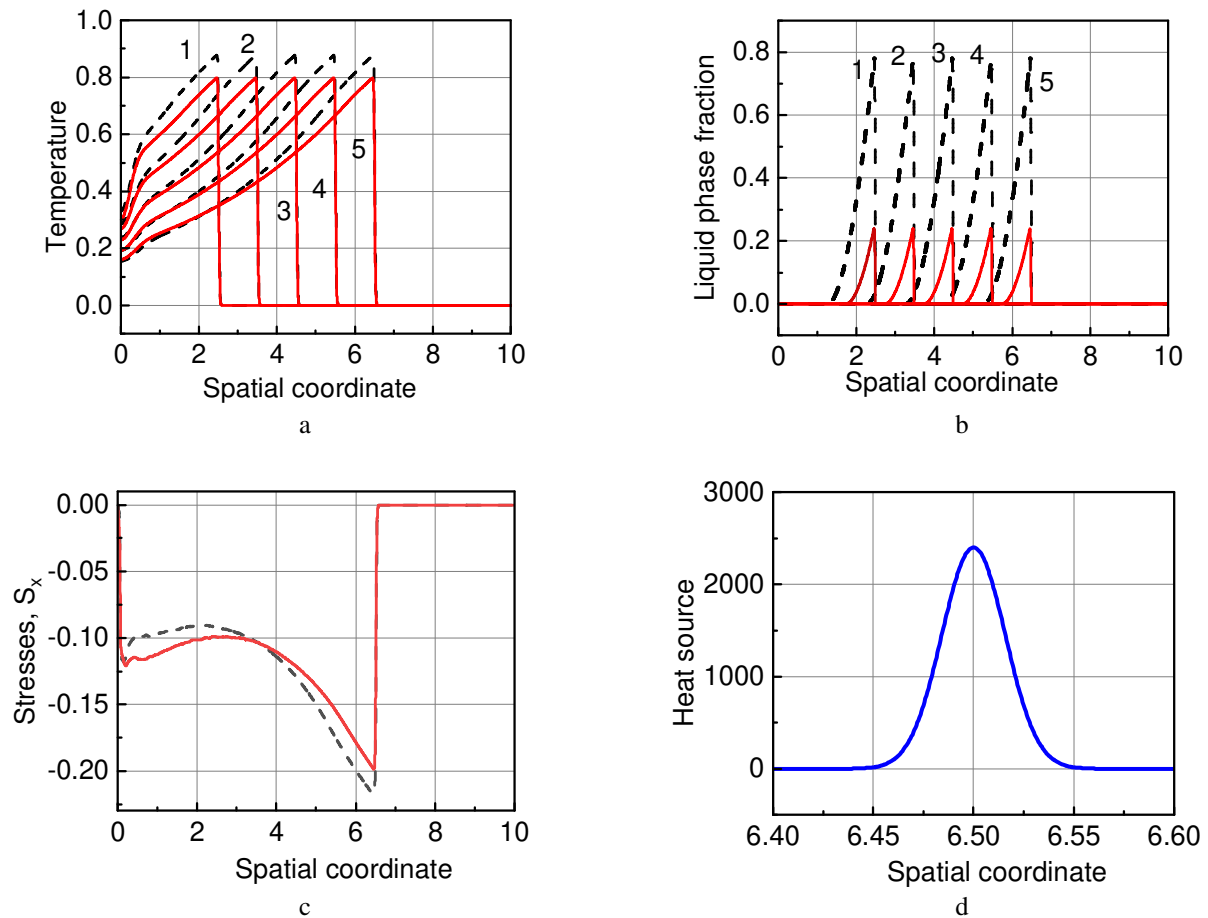
Fig.3. Tepperature (a) and liquid phase fraction (b) distributions for different time moments, τ: $1 - 2.4 \cdot 10^{-2}$; $2 - 3.4 \cdot 10^{-2}$; $3 - 4.4 \cdot 10^{-2}$; $4 - 5.4 \cdot 10^{-2}$; $5 - 6.4 \cdot 10^{-2}$. Stresses (c) for time $\tau = 6.4 \cdot 10^{-2}$ and energy in heat source (d) distributions. Solid lines – coupled problems; dotted lines – non-coupled problems.

Acknowledgements

5. References

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