A behavior model of the viscoelastic system with a melting component under load

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Abstract. A numerical investigation of a stressed-strain state powder mixture with a melting component is carried out for the conditions of one-axial loading and nonstationary heating. The state of plane stress was assumed. The influence of the coupling between thermal and mechanical processes on temperature, stress and strains fields was investigated.

1. Introduction
The influence of mechanical stresses on temperature fields and rates of solid-phase chemical reactions has been studied by many authors. Based on experimental data similar to [1-3] theoreticians suggest mathematical models taking into account the features of solid-phase reactions (a heterogeneous character of the reactions, the important role of transport processes and the interrelation between various physical phenomena) [4]. However, the coupled processes of a different physical nature are not included in traditional models. Nevertheless, it was shown in [5-7] that coupling between mechanical, thermal and chemical processes leads to features in the stressed-strain state and reaction front propagation.

This work investigates the stressed-deformed reactive substance state based on melting one of the components, coupling of deformation, temperature and concentration fields.

2. Problem formulation
The fixed plate of the reactive substance under external uniaxial tension is considered. We assume the reactive substance is the compaction of a metallic powder into a plate form. Length of the plate $L_x$, width $L_y$, height $L_z$ and conditions $L_z \ll L_x, L_y$ are satisfied. The chemical reaction and heating propagates along the X-axis. The external loading direction is perpendicular to that of chemical reaction propagation. We consider the melting one of a component powder mixture. The exothermal reaction is assumed to describe summary schema $B \rightarrow A$.

To estimate a stressed-deformed state of the plate and the influence of coupling field on a solid-phase reaction we consider the uniaxial tension problem (with a chemical reaction), which consists of two parts [7]. These parts are independently solved.

The first part of the problem includes the energy equation for a viscoelastic body [8], the initial and boundary conditions

$$\sigma_{ij, t} + c_v \rho \frac{\partial T}{\partial t} = \nabla \cdot \lambda \nabla T + Q \phi(\eta, T) - 3K T \alpha \frac{\partial E_{ik}}{\partial t},$$

(1)
\[ t=0: T=T_0, x=0: -\lambda \frac{\partial T}{\partial x} = q(t), \quad y=0: \frac{\partial T}{\partial y} = 0, \quad y=L_y: \frac{\partial T}{\partial y} = 0, \quad (2) \]

where \( c_e, \rho \) and \( \lambda_T \) are the effective heat capacity, density and thermal conductivity, \( T \) is the plate temperature, \( q(t)=q_0 f(t) \) is an external heat source, \( q_0 \) is the maximal density of the heat flux; \( x \) and \( y \) are space coordinates, \( \varepsilon_{kk}=\varepsilon_{xx}+\varepsilon_{yy}+\varepsilon_{zz} \) is the first invariant of the strain tensor, \( \alpha_T \) is a thermal expansion coefficient, \( K \) is an isothermal bulk modulus, \( \sigma_{ij}, \varepsilon_{ij} \) are the components of stress and strains tensors. We consider that the heat source varies with the time. Let us consider the heat capacity, density and thermal conductivity and mechanical properties dependence on temperature and compound, for example

\[ \varepsilon_3 = \varepsilon_1 \rho_3 + \varepsilon_2 \rho_2 + \varepsilon_1 \rho_1, \]

where \( \chi_{1,2,3} \) are volume fraction of 1, 2 component (reactants) and reaction product, respectively.

The melting of one of the components is assumed as

\[ T_{m}(T_{m} - T + \delta(T - T_m)), \]

where index “0” is the solid properties, \( T_m \) is the melting temperature, \( L_m \) is the heat of phase transition, \( \delta \) is the Dirac delta function.

The present model includes a simple linear viscoelastic model (Maxwell body). The deviatoric stress-strain relation for a Maxwell body is \[ e_{ij} = \frac{1}{\mu} \sigma_{ij} + \frac{1}{2\eta_v} \dot{\varepsilon}_{ij}, \]

where \( e_{ij}, \dot{\varepsilon}_{ij} \) are the dimensional deviatoric strain and stress tensors, respectively, \( \mu \) is the shear modulus, \( \eta_v \) is the viscosity of the viscoelastic solid.

The second part of the problem describes the mechanical equilibrium of the plate. We consider stressed-deformed state of the plate as a plane stress state. So, \( \sigma_{zz} = 0 \) and two equilibrium equations are \[ \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0, \quad \frac{\partial \sigma_{yy}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} = 0. \quad (3) \]

The complete stress-strain relation for a Maxwell body may then be stated \[ \frac{\partial \sigma_{xx}}{\partial t} + \frac{\mu}{\eta} \sigma_{xx} = 2\mu \frac{\partial e_{xx}}{\partial t} + 3\lambda \frac{\partial e_{kk}}{\partial t} - 3K \left[ \frac{\partial \varepsilon_{kk}}{\partial t} - \frac{\mu}{\eta} (\varepsilon_{kk} - \omega) \right], \]

\[ \frac{\partial \sigma_{yy}}{\partial t} + \frac{\mu}{\eta} \sigma_{yy} = 2\mu \frac{\partial e_{yy}}{\partial t} + 3\lambda \frac{\partial e_{kk}}{\partial t} - 3K \left[ \frac{\partial \varepsilon_{kk}}{\partial t} - \frac{\mu}{\eta} (\varepsilon_{kk} - \omega) \right], \]

\[ \frac{\partial \sigma_{xy}}{\partial t} + \frac{\mu}{\eta} \sigma_{xy} = 2\mu \frac{\partial e_{xy}}{\partial t} \]

\[ 0 = 2\mu \frac{\partial e_{zz}}{\partial t} + 3\lambda \frac{\partial e_{kk}}{\partial t} - 3K \left[ \frac{\partial \varepsilon_{kk}}{\partial t} - \frac{\mu}{\eta} (\varepsilon_{kk} - \omega) \right] \]

Also, we use the equation of compatibility of strains

\[ \frac{\partial^2 e_{xx}}{\partial x^2} + \frac{\partial^2 e_{xy}}{\partial x \partial y} = \frac{\partial^2 e_{xy}}{\partial y^2} \]

We assume that uniform load \( P \) along the \( y \) axis was applied to the ends of the plate at \( x=0 \) and \( x=L_x \). The boundaries of the plate are free at \( y=0 \) and \( y=L_y \):

\[ x=0: x=L_x: \sigma_{xx} = 0, \quad \sigma_{xy} = P, \quad \sigma_{yy} = 0; \]

\[ y=0, y=L_y: \sigma_{xx} = 0, \quad \sigma_{yy} = 0, \quad \sigma_{xy} = 0. \]
The strain tensor components follow from (4). The problem was solved numerically. The differential equations included into system (1)-(3) were approximated by difference equations; the resulting system of linear algebraic equations was solved by a sweep method. In our calculations, we determine the temperature, concentration, stress and strains distributions in the plate at different time instants by varying the physical parameters.

We consider that the reactive plate consists of metal powder Al+Ni. All calculations presented further were carried out for parameters [10]:

1) \( \text{Al}_2\text{O}_3 \): \( \lambda_p = 35 \text{ W/(m·K)} \), \( \rho_p = 3750 \text{ kg/m}^3 \), \( c_p = 858 \text{ J/(kg·K)} \), \( \alpha_{T,p} = 8 \cdot 10^{-6} \text{ K} \), \( \nu_p = 0.33 \), \( E_p = 370 \text{ GPa} \).

2) Ni: \( \lambda_m = 91 \text{ W/(m·K)} \), \( \rho_m = 8902 \text{ kg/m}^3 \), \( c_m = 416 \text{ J/(kg·K)} \), \( \alpha_{T,m} = 13.5 \cdot 10^{-6} \text{ K} \), \( \nu_m = 0.3 \), \( E_m = 200 \text{ GPa} \).

The effective heat capacity satisfies the mixture rule (this follows from thermodynamics)

\[
\rho_c = \rho_p \eta + \rho_m (1 - \eta).
\]

3. Results and Discussion

Figure 1 shows a special distribution of temperature, the first invariant of the stress tensor at the moment \( t = 0.015 \) and maximum temperature of the plate. We can observe the impulse character of the heating plate (Figure 2a): at first, the maximum temperature increases smoothly until the end of impulse \( t_i \), then the temperature decreases for some time, that is, until \( t_p \), next impulse leads to further heating (curve 1, Figure 1a) or the heat release due to increased active chemical conversion (curves 2 and 3, Figure 1a). The inhibition of the reaction product layer results in slower increasing of temperature due to the chemical reaction (curve 3, Figure 1a, c).

Figure 1. Maximum temperature of the plate (a) and spatial distributions of the plate temperature (b), the temperature (c) and the first invariant of the stress tensor (d) along x-axis at the moment \( t = 0.015 \): \( t_i = t_p = 5 \cdot 10^{-3} \text{ c}, n = 10, q_0 = 10^7 \text{ W/m}^2 \), \( P = 1 \text{ GPa} \). 1. The chemical reactions are absent; 2. The first-order reaction; 3. The inhibition of the reaction products is taken into account in the kinetic function (\( m_0 = 2, n_0 = 0 \)).
The assumption of coupled thermal and deformation fields leads to arising of a non-unidimensionality border effect. The temperature profile has a ‘bend’ due to mechanical dissipation and interaction of thermal and mechanical processes (Figure 1b).

If we consider only thermal stresses, the maximum mechanic stresses reach a value of 1.5 GPa (curves 2, 3, Figure 1d). The concentration expansion of reaction products leads to an increase of stress, that of magnitude becomes comparable to the applied external load (curve 2, Figure 1d).

4. Conclusion

A model of uniaxial tension plate heating with allowance for interaction of thermal and mechanical processes, as well as the concentration expansion was proposed in the paper. As the example of Ni+Al powder system shows, the thermal and mechanical coupling processes lead to non-unidimensionality border effects and decrease of the maximum temperature. Also it was shown that the internal stresses caused by a chemical reaction can reach values comparable to the applied external load, taking into account the coupling of thermal, concentration and mechanical fields.

Acknowledgments

This work was supported by state project ‘Development of physical principle of metallic and composite material designing with multimodal internal structure’ № 01201350716.

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