Kinetics of powder layer shrinkage during electron-beam treatment

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Abstract. When layerwise synthesis of new material occurs, only thin surface area, thin melt film or thin powder layer undergo essential changes. To describe the behaviour of thin layer where temperature and composition change, a model similar to shallow-water theory is suggested. The equations for thin layer behaviour are deduced for the Maxwell model of viscoelastic body in the approximation of incompressibility. The hydrodynamic part of the problem is coupled with thermal-kinetical one.

1. Introduction

Electron-beam (EB) technologies are interesting for development of manufacturing and for investigation in the directions involving the modification of material properties and its surfaces. Recent applications are connected with additive manufacturing [1]. Thermophysical phenomena determining the additive manufacturing results are the same [2] that take a place in the processes of laser and electron beam welding, surfacing and surface treatment [3]. However, there are the features in the laser and electron beam energy absorption by material. When EB acts on the powder layer, practically total energy has been used for the heating. Because EB-treatment happens in the vacuum chamber (without inert atmosphere or air), the result of the technological process is a more predictable. Generally, there are several types of technologies of EB- material synthesis: powder layer has been deposited preliminarily on the substrate and then it is treated by EB; powder enters in the melting pool traversing EB; the metallic wires have been used instead powder jet; EB acts locally to initiate the melting and intermixing between different materials or new phase formation in the heated area, and etc. In any case, the evolutions of the composition and the structure of treated material are very complex.

In additive manufacturing applications, it is necessary to know and predict the possible shrinkage of a powder layer during Selective Laser or Electron Beam Melting. This phenomenon in different technologies can be linear [4] or nonlinear in connection with nonlinear thermal conductivity or phase transitions [5]. There are many physical factors that affect the densification of the products during EB - sintering of metallic powders. It is not possible practically to take into account all phenomena in generalized model because different physical phenomena are characterized by different spatial and temporal scales. The set of limiting phenomena depends on the materials under study. Thermal-kinetical models of surface EB-treatment were suggested in [6-8]. Even in the simplest approximation (without hydrodynamics of melting pool and without rheological features of heterogeneous media),
similar models give reliable change if powder layer thickness with the temperature at the variation of EB-parameters. The kinetic laws can be constructed based on Phase-field method [9] and lattice Boltzmann equation method [10].

In this paper, new approach is suggested to describe the evolution of thin surface layer under traveling EB-action.

2. Key equations

When layerwise synthesis of new material occurs, only thin surface area, thin melt film or thin powder layer undergo essential changes. In this thin area, the structure, composition and properties form. To describe the behavior of this thin area, one can use the approximation typical for the shallow-water theory [11]. However, the pure (classical) hydrodynamic model is not suitable here because solid and liquid phases and their mixture present in this traveling area simultaneously.

We assume that the behavior of the mixture consisting of powders, melt, and new solid and liquid phases and containing the pores can be described on the base of Maxwell model of viscoelastic body [12]. In this model, the components of deviators of stress and strain tensors are connected by relations

$$ e_{ij} = \frac{1}{2\mu} \frac{ds_{ij}}{dt} + \frac{1}{2\eta_v} s_{ij}, $$

and the usual equality

$$ \sigma_{kk} = 3K(e_{kk} - \omega) $$

(2)

takes a place. Here, $ e_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk}$, $ s_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk}$, $ \mu $ is the shear module, $ K $ is the bulk module, $ \eta_v $ is the viscosity, the function $ \omega $ depends on the temperature, composition and porosity.

Substituting (2) into (1), we obtain

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

(3)

Here, $ \lambda = K - \frac{2}{3}\mu $. Viscosity depends on the temperature, composition and porosity. If $ \eta_v \rightarrow \infty $, we come to the model of solid body. If $ \eta_v \rightarrow 0 $, we obtain ideal liquid.

Motion and continuity equations are usual for hydrodynamics

$$ \rho \frac{dv}{dt} = F + \nabla \cdot \sigma, $$

(4)

$$ \frac{dp}{dt} + \rho \nabla \cdot v = 0. $$

(5)

Energy equation in the form of thermal conductivity equation contains terms connecting with viscous dissipation, coupling and sources due to chemical reactions

$$ \sigma \cdot \frac{de}{dt} + c_e \rho \frac{dT}{dt} = \nabla \cdot \lambda_T \nabla T + W - 3K \alpha_T \frac{d\varepsilon_{kk}}{dt}. $$

(6)

Here, $ c_e $ is the heat capacity for constant strains, $ \lambda_T $ is effective thermal conductivity, $ \alpha_T $ is the linear thermal expansion coefficient, $ \rho $ is the density, $ v $ is the velocity vector.

Further we take into account that metals have high thermal conductivity, only thin layer can melt, the $ OX $ and $ OY $ axes of Cartesian coordinate system are directed along the treated surface, the $ OZ $ axis is perpendicular to this surface and is directed upward.

3. Equations for thin layer

Firstly, we construct thermal conductivity equation for metallic substrate with the preliminary deposited coating. The properties of the substrate with the thickness $ h_A $ have the index “A”. We use the index “B” for the coating with small thickness $ h_B = h_B(t,x,y) $. The contact between the
substances is assumed as ideal. In the first approximation, the substrate stays solid and immovable. The external heat source connecting with travelling EB inter into the boundary condition

$$\lambda_B \frac{\partial T}{\partial z} + c_B \rho_B w(T - T_0) = q_0 f(x, y; t) = W_{ext}.$$  

Due to high thermal conductivity of metals and small thickness of the coating, we integrate the equation (6) along OZ axis. As a result, we obtain the equation

$$U \frac{\partial T}{\partial t} + c_B \rho_B h_B \left[ u' \frac{\partial T}{\partial x} + v' \frac{\partial T}{\partial y} \right] = \frac{\partial}{\partial x} \left( W \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( W \frac{\partial T}{\partial y} \right) + W_{ext} + h_B W(T) - H(x, y, t),$$

where

$$U = c_A \rho_A h_A + c_B \rho_B h_B; \ W = \lambda_A h_A + \lambda_B h_B,$$

and convective velocities contain additive terms, connecting with coating thickness evolution:

$$u' = u + \frac{\lambda_B}{c_B \rho_B} \frac{1}{h_B} \frac{\partial h_B}{\partial x}; \ v' = v + \frac{\lambda_B}{c_B \rho_B} \frac{1}{h_B} \frac{\partial h_B}{\partial y}.$$  

The term $H(x, y, t)$ depends on the solution of mechanical part of the problem. Hence, secondly, we should find the equations describing the evolution of the coating thickness. Thermal-kinetical model [8] uses the kinetic equations for thickness $h_B$, porosity $\theta$ and the relation

$$\rho = \rho_S (1 - \theta).$$

Taking into account the relations

$$\frac{d\varepsilon_{ij}}{dt} = \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right),$$

where $v_1 = u, v_2 = v, v_3 = w; \ x_1 = x, x_2 = y, x_3 = z$, we can write

$$\frac{d\varepsilon_{kk}}{dt} = \nabla \cdot \mathbf{v} = \frac{1}{\rho} \frac{d\rho}{dt}.$$  

For porous substance, we can assume

$$\varepsilon_{kk} = \ln \frac{\rho_0}{\rho} = \ln \frac{1 - \theta_0}{1 - \theta},$$

where index “0” relates to initial state.

For EB-sintering powder mixtures, the medium models used for hot pressing [13] are suitable. For viscoelastic body of Maxwell type, if medium is incompressible, we come to equations

$$\frac{d\sigma_{ij}}{dt} + \frac{\mu}{\eta_v} \sigma_{ij} = 2\mu \frac{d\varepsilon_{ij}}{dt} + \frac{K\mu}{\eta_v} (\varepsilon_{kk} - \omega) - \frac{K}{\eta_v} \frac{d\omega}{dt} \delta_{ij}. \quad (8)$$

Neglecting the velocity component $w$ in comparison with $u, v$ and using usual dynamical condition, we can find

$$\sigma_{zz} = p g (\zeta - z),$$

where $\zeta = \zeta(t; x, y)$ is the coordinate of the free boundary.

Then substituting (9) into (8) for $i = j = z$, we obtain

$$\rho g \frac{d\zeta}{dt} + \frac{\mu}{\eta_v} p g (\zeta - z) = 2\mu \frac{d\varepsilon_{zz}}{dt} + \frac{K\mu}{\eta_v} (\varepsilon_{kk} - \omega) - \frac{K}{\eta_v} \frac{d\omega}{dt}. \quad (10)$$

Now we can integrate this equation with $z$ using the kinematical conditions:

$$w = 0 \text{ for } z = 0 \text{ and } \frac{\partial \zeta}{\partial t} + u \frac{\partial \zeta}{\partial x} + v \frac{\partial \zeta}{\partial y} = w \text{ for } z = \zeta.$$
\[ \rho g \zeta \frac{\partial \zeta}{\partial t} + \frac{\mu}{\eta_v} \rho g \frac{\zeta^2}{2} = 2\mu \left[ \frac{\partial \zeta}{\partial t} + u \frac{\partial \zeta}{\partial x} + v \frac{\partial \zeta}{\partial y} \right] + \frac{\mu}{\eta_v} \zeta \left( p - K \frac{do}{dt} \right), \]  

(11)

where \( p = \frac{\sigma_{kk}}{3} \).

Continuity equation \( \nabla \cdot \mathbf{v} = 0 \) together with (10) gives known equation

\[ \frac{\partial \zeta}{\partial t} + \frac{\partial}{\partial x} (\zeta u) + \frac{\partial}{\partial y} (\zeta v) = 0. \]  

(12)

The final equation system includes (12) for \( \zeta \), (11) for \( p \), the equations

\[ \frac{d\sigma_{xx}}{dt} + \frac{\mu}{\eta_v} \sigma_{xx} = 2\mu \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + \frac{\mu}{\eta_v} \sigma_{yy} - K \frac{do}{dt}, \]

\[ \frac{d\sigma_{yy}}{dt} + \frac{\mu}{\eta_v} \sigma_{yy} = 2\mu \left( \frac{\partial v}{\partial y} + \frac{\partial u}{\partial x} \right) + \frac{\mu}{\eta_v} \sigma_{xx} - K \frac{do}{dt}, \]

\[ \frac{d\sigma_{xy}}{dt} + \frac{\mu}{\eta_v} \sigma_{xy} = \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \]

for stress tensor components and equations

\[ \rho \left( \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y}, \]

\[ \rho \left( \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = \frac{\partial \sigma_{yy}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} \]

for velocities.

For particular cases, we can simplify the equations.

The more rigorous dynamical conditions should include the force of surface tension.

It is obvious that \( h_B = \zeta \). In this approximation the density \( \rho \) is the function of the temperature, composition and porosity similarly to the function \( \omega \). To study the composition evolution, it is necessary to formulate special subproblem usual for macro kinetics and chemical hydrodynamics.

4. Conclusion

So, the model is formulated for the description of thin layer behavior during the electron beam treatment. It is shown that mechanism of heat transfer appears connecting with treated layer evolution. It is necessary further to determine the laws for viscosity evolution with the temperature especially near the melting temperature, where rheological behavior of the mixture changes. For various technological conditions, the model could be modified similarly to [7,14].

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