Surface layer evolution under the external heating

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Abstract. Generalized equation system is written to describe the surface layer evolution under electron beam action. Chemical reactions and porosity evolution are taken into account. The model was used to describe the electron beam treatment of thin layer with varied thickness. The review is made for some previous particular models of electron beam surface treatment with chemical reactions and shrinkage. It was pointed that the model permits the existence of self-sustaining regimes and quasi-stationary technology regimes.

1. Introduction

Electron-beam and laser technologies are interested for the development of new materials production and for the treatment and modification of the surfaces of metals and alloys. The last technologies connect immediately with additive manufacturing [1]. Thermo-physical phenomena determining the details properties in additive manufacturing based on electron and laser beam employment are typical for high temperature technologies [2]. However, in powder 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 or nonlinear in connection with nonlinear thermal conductivity, nonlinear absorptance or phase transitions, porosity evolution [3, 4]. There are many physical factors that affect the densification of the products during sintering of metallic powders [5, 6]. 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 [7]. Known simplified thermal models of surface treatment and selective laser melting describe some effects [8, 9]; there are laser welding models [10], where reliable changes of melting pool due to nonlinear surface tension have been modeled. Thermal-kinetic models of surface layer evolution during EB-treatment were suggested in [11-13]. Porosity evolution in the heated zone is taken into account explicitly in [14], and new approach is suggested in [15] to describe the evolution of thin surface layer under traveling energy source action.

In this paper, the interrelation between chemical reactions and mechanical processes are taken into account to describe the surface layer formation on substrate under moving electron beam action. The model generalizes the previous investigations [11-16].

2. Key equations

Similarly to [15, 16], we assume that the evolution of the mixture consisting of powders, melt, and new solid and liquid phases and containing the pores can be described by Maxwell model of viscoelastic body [17]. In this model, components of deviators of stress s_{ij} and strain e_{ij} tensors are connected by relations

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

and the usual relation between first invariants of stress and strain tensors

$$\sigma_{kk} = 3K(\varepsilon_{kk} - \omega) \tag{2}$$

takes a place. Here

$$e_{ij} = \varepsilon_{ij} - \frac{1}{3}\varepsilon_{kk}\,; \; s_{ij} = \sigma_{ij} - \frac{1}{3}\varepsilon_{kk}\,; \tag{3}$$

μ is the shear module, K is the bulk module, η_V is the viscosity; the function ω depends on the temperature and composition

$$\omega = 3\left[\alpha_T(T - T_0) + \sum_{k=1}^{n}\alpha_k(C_k - C_{k0})\right], \tag{4}$$

where α_T is the thermal expansion coefficient, C_k – mass concentrations of species (reagents and products), α_k are concentration expansion coefficients; index "0" relates to the initial state.

Substituting (2) into (1) we obtain

$$\frac{d\sigma_{ij}}{dt} + \frac{\mu}{\eta_v}\sigma_{ij} = 2\mu\frac{d\varepsilon_{ij}}{dt} + \delta_{ij}\left[\lambda\frac{d\varepsilon_{kk}}{dt} - K\frac{d\omega}{dt} + \frac{K\mu}{\eta_v}(\varepsilon_{kk} - \omega)\right], \tag{5}$$

where λ, μ – Lame coefficients; $K = \lambda + \frac{2}{3}\mu$ – bulk module; η_V – viscosity.

If $\eta_V \to \infty$, we come to the model of solid body. If $\eta_V \to 0$, we obtain ideal liquid. If we take

$$\eta_V = \eta_V(T, \theta), \; \mu = \mu(T, \theta), \; \lambda = \lambda(T, \theta), \tag{6}$$

where θ – is the porosity changing during shrinkage, then rheology of the reacting mixture will depend on temperature and composition evolution.

Motion and continuity equations are usual for hydrodynamics:

$$\rho\frac{d\mathbf{v}}{dt} = \mathbf{F} + \nabla\cdot\boldsymbol{\sigma}, \tag{7}$$

$$\frac{d\rho}{dt} + \rho\nabla\cdot\mathbf{v} = 0. \tag{8}$$

Energy equation in the form of thermal conductivity equation will contain the terms connecting with viscous dissipation, coupling effect and energy sources due to chemical reactions happen during surface treatment

$$\boldsymbol{\sigma}\cdot\frac{d\boldsymbol{\varepsilon}}{dt} + c_\varepsilon\rho\frac{dT}{dt} = \nabla\cdot(\lambda_T\nabla T) + W - 3KT\alpha_T\frac{d\varepsilon_{kk}}{dt} \tag{9}$$

Here c_ε is the heat capacity for constant strains; λ_T is effective thermal conductivity coefficient; ρ is the density; $\mathbf{v}$ is the velocity vector. Thermal properties depend on porosity also, and some kinetic law should be formulated for porosity evolution

$$\frac{d\theta}{dt} = \varphi(\theta, T, \sigma_{kk}) \tag{10}$$

The term W includes chemical heat release and the heat from external heating, if energy absorption takes a place in the volume. Chemical source is the sum

$$W_{ch} = \sum_{i=1}^{r} Q_i \varphi_i \qquad (11)$$

where Q_i and φ_i - heats and rates of the reactions, $i=1,2,...,r$.

Molar concentrations of species (connecting linearly with mass concentrations) follow from the equation system of chemical kinetics corresponding to the stages of chemical reaction under study. Boundary conditions correspond to experimental situation.

3. Reactions in thin layer

If reaction occurs in thin layer placed on some substrate and external source is developed in line and moves in the direction *0x* of Cartesian coordinate system, we can assume $\varepsilon_{yy} = 0$; $\sigma_{zz} = 0$ and other components of strain and stress tensor depend on coordinate *x* only. In his case we obtain four equations from (5) and equilibrium equation (only one equilibrium equation remains here if inertia forces are negligible small) to find the values $\varepsilon_{xx}, \varepsilon_{zz}$ and σ_{xx}, σ_{yy} depending on temperature and composition. Then integrating the thermal conductivity equation along the thickness we obtain

$$U \frac{\partial T}{\partial t} + c_B \rho_B h_B u' \frac{\partial T}{\partial x} = \frac{\partial}{\partial x}\left(W \frac{\partial T}{\partial x}\right) + W'_{ext} + h_B W(T) - H(x,t), \qquad (12)$$

where the term $H(x,y,t)$ depends on the solution of mechanical part of the problem

$$H(x,t) = \sigma_{xx} \frac{d\varepsilon_{xx}}{dt}(h_B + h_A) + 3BT \frac{d\varepsilon_{kk}}{dt} \qquad (13)$$

and designations

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

$$u' = u + \frac{\lambda_B}{c_B \rho_B} \frac{1}{h_B} \frac{\partial h_B}{\partial x}, \; B = K_A \alpha_{TA} h_A + K_B \alpha_{TB} h_B$$

are introduced. Index "A" relates to the substrate, "B" relates to the treated layer; where h_A and h_B are their thicknesses.

For porous substance, we can assume [15]

$$\varepsilon_{kk} = ln \frac{\rho_0}{\rho} = ln \frac{1-\theta_0}{1-\theta} \qquad (14)$$

where $\rho = (\rho_A h_A + \rho_B h_B)/(h_A + h_B)$ – is the averaging density. The density $\rho_B = \rho_S(1-\theta)$ depends on the composition changing during reaction.

Assuming that mass does not change during the treatment with the reactions in condensed phases we can write simple relation for the thickness of layer B:

$$h_B = h_{B0} \frac{1-\theta_0}{1-\theta}. \qquad (15)$$

Particular variants of one-dimensional problems describing surface layer evolution were investigated in [11-16, 18 and 19]. So, the model of synthesis process in the layer containing *TiAl₃* and *Ti*, placed on substrate made of *Fe* and heated by moving electron beam was suggested in [16]. Shrinkage process did not analyze. The paper [18] was devoted to the study of coupling problem, where

mechanical stresses accompanying the chemical reactions in the system $TiNi_3 + Ti$ were taken into account. Shrinkage of powder layer from Ti-Nb alloy in two-dimensional formulation was analyzed in [14], where the melting process was modeled in term of two-phase zone. The intermixing of mixture from *Ni* and *Al* with substrate alloyed by electron-beam was analyzed in [19].

The question appears: "Will possible self-sustaining regime in reacting mixture initiated by electron-beam?" It was shown in [16] for simple formulation that self-sustaining combustion regime can appear, however it was not detected there numerically due to high heat losses to substrate.

When electron beam moves along the surface of large size, quasi-stationary regime establishes. Quasi-stationary models were analyzed in laser and electron-beam welding, for example, it is described in [20]. Here going to the coordinate system connecting with moving electron beam we come to nonlinear thermal conductivity equation with coefficients depending on mechanical properties and porosity. This problem demands a special investigation.

4. Conclusion

So, generalized equation system is written to describe the surface layer evolution under electron beam action. Chemical reactions and porosity evolution are taken into account. The equations were simplified for thin layer of variable thickness. It was shown that previous particular models of electron beam surface treatment with chemical reactions and shrinkage are contained in general model. It was pointed that the model permits the existence of self-sustaining regimes and quasi-stationary technology regimes that should be investigated specially.

Acknowledgments

References
[1]   Beaman J J (Chair), Atwood C, Bergman T L, Bourell D, Hollister S, Rosen D 2004 WTEC Panel Report on Additive/subtractive manufacturing research and development in Europe, (World Techn. Ev. Center, Inc. 2809 Boston Street, Suite 441. Baltimore, Maryland 21224) 136
[2]   Nicholas P L et al 2014 *Sustainable Design and Manufacturing* **7** 668
[3]   Sercombe T B and Hopkinson N 2006 *Advanced engineering materials* **8** 260
[4]   Ranogajec J et al 2000 *Ceramics – Silikáty* **44** 71
[5]   Herderick E 2011 *Materials Science and Technology* (MS&T) ASM International 176252
[6]   Lawrence E et al 2012 *Mater. Sci. Technol.* **28** 1
[7]   Rishi Ganeriwala, Tarek I Zohdi 2014 *Procedia CIRP* **14** 299
[8]   Tiebing Chen,Yuwen Zhang 2007 *Appl. Phys.* **86** 213
[9]   John Romano et al 2015 *Procedia Manufacturing* **1** 238
[10]   Isaev V I et al 2017 *AIP Conference Proceedings* **1893** 030108
[11]   Knyazeva A G et al 2007 *Physical mesomechanics* **10** 207
[12]   Knyazeva A G, Pobol I L, Demidov V N 2016 *Additive Technologies IOP Conf. Series: Materials Science and Engineering* **140** 012021
[13]   Knyazeva A G, Bookrina N V 2003 *Materials of 12th International conference on radiation physics and chemistry of inorganic materials* (23–27 September, 2003, Tomsk: TPU). 167
[14]   Knyzeva A G and Sharkeev Yu P 2017 *AIP Conference Proceedings* **1893** 030105
[15]   KnyazevaA G 2016 *J. Phys.: Conf. Ser.* **754** 042009 https://doi.org/10.1088/1742-6596/754/4/042009
[16]   Sorokova S N and Knyazeva A G 2008 *Theor. Foundations of Chemical Engineering* **42** 443
[17]   Boley B A and Weiner J H 1960 Theory of Thermal Stresses (Wiley, New York) 540
[18]   Sorokova S N and Knyazeva A G 2010 *Theor.Foundations of Chemical Engineering* **44** 172
[19]   Knyazeva A G and Kryukova O N 2017 *J. Phys.: Conf. Ser.* **899** 072001 https://doi.org/10.1088/1742-6596/899/7/072001