IOP Conf. Series: Materials Science and Engineering **140** (2016) 012021 doi:10.1088/1757-899X/140/1/012021

Mathematical modelling of thermal and kinetic phenomena in electron-beam technologies

A G Knyazeva[1,3], I L Pobol[2], V N Demidov[1]
[1] Tomsk Polytechnic University, Tomsk, Russia
[2] Physical-technical Institute of the National Academy of Sciences of Belarus, Minsk
3 Institute of Strength Physics and Materials Science of the Siberian Branch of the Russian Academy of Science, Tomsk, Russia

E-mail: anna-knyazeva@mail.ru

Abstract. The article presents a scheme for constructing models using kinetic laws for additional parameters. The work describes the example of the model of electro-beam treatment of a material with a coating. The study uses the simple kinetic law for powder layer evolution due to shrinkage. The model takes into account the melting of powder layer and substrate. The numerical solution gives the temperature field, evolution of the molten pool, the heat affected zone and the surface relief for different moments of time. The results depend on the treatment rate and electron beam energy.

1. Introduction

Electron-beam technologies are interesting for development of manufacturing and for investigation in the directions involving the modification of material properties and its surfaces [1–3]. Recent applications are connected with additive manufacturing [4]. The viability of laser-based and electron-beam-based additive manufacturing has been successfully demonstrated for titanium and nickel-based alloys, for stainless steel. etc. Thermophysical phenomena determining the additive manufacturing results are the same [5] that take a place in the processes of laser and electron beam welding, build up welding and surface treatment [6].

Additive methods for producing metallic parts are developed in the directions of powder and wire employment as green materials. There are technologies, where layer build-up happens due to the feeding of a wire or powder into the heated zone or into the melt formed by laser or electron beams. Another way of additive layer manufacturing using metal powder compositions uses the fusing of layers by scanning beam of small diameter. Note that electron-beam additive manufacturing is characterized by the building-up velocity of 120 cm^3/h, which is higher than 2-20 cm^3/h for similar laser machines. In addition, sintering of chemically active metals (particularly, titanium and their alloys) in vacuum is cheaper than that for corresponding laser process in protective gas environment.

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 [7] or nonlinear in connection with nonlinear thermal conductivity or phase transitions [8]. There are many physical factors that affect densification of products during sintering [8, 9]. These processes play a significant role when homogeneity of mechanical and physical properties of synthesized material is required in the direction normal to the directions of heated zone propagation and article production. In addition to the modelling of shrinkage during solid freeform

fabrication [10] based on FEM (Finite-Element Method), it is important to study the models, where the shrinkage process can be described by kinetic laws based on physical regularities that are typical for them [11, 12].

Because the thickness of consecutive powder layers is small in comparison with specific heat scale and detail size and one powder layer includes only several particles, the approach schematically depicted in Figure 1 is methodologically correct and will yield prognostic models.

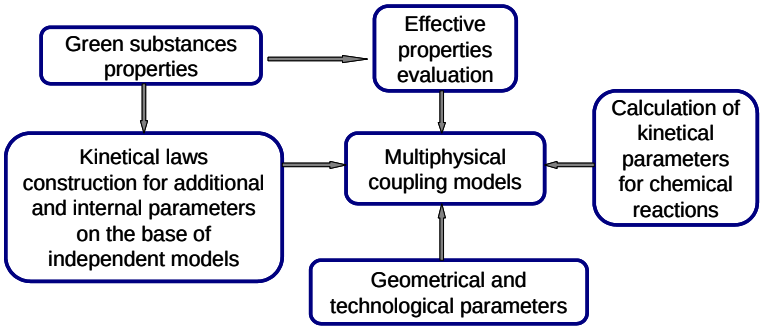


Figure 1. Conditional scheme for coupling models construction

Note that the construction of kinetic laws is possible at meso level, when the observation after individual particle behaviour is ensured. Here, the Phase-field method [13] and lattice Boltzmann equation method [14] are suitable. Unfortunately, the authors of similar works do not suggest the generalized formulae. Kinetic parameters for chemical reactions can be found using thermodynamics, quantum chemistry, molecular methods or experiment. Effective properties are quite structure-sensitive, and there are numerous theoretical approaches in micromechanics and thermal physics for their calculation.

Here, we demonstrate some features of the models with kinetic laws for evolution of powder layer thickness.

2. Thermophysical model formulation

A mathematical model of surface treatment of the plate (with preliminarily deposited powder layer) by scanning electron beam developed in the line can be presented in the form [15].

$$(c\rho)_{eff}\frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(\lambda_{eff}\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(\lambda_{eff}\frac{\partial T}{\partial y}\right)+\frac{q_{eff}}{h_b}f(x,y,t)-\sigma\varepsilon_{eff}\left(T^4-T_W^4\right) \quad (1)$$

$$x=0,H_x:\ \frac{\partial T}{\partial x}=0\,,\ y=0,H_y:\ \frac{\partial T}{\partial y}=0\,, \quad (2)$$

$$t=0:T=T_0\,, \quad (3)$$

where

$$f(x,y,t)=exp\left[-\frac{(x-Vt)^2}{R_0{}^2}\right],|y|\le h_y,\ f(x,y,t)=0,|y|>h_y\,,$$

h_y is the scanning width, H_x, H_y are the sizes of the plate along x and y directions, R_0 is the electron beam radius; σ is Stefan-Boltzmann constant; $\varepsilon_{eff}=(\varepsilon_1+\varepsilon)/h_b$ is effective emissivity; q_{eff} is the effective source power density of (with regard to volume absorption). Effective thermophysical properties are averaged along the thickness of the layers

$$(c\rho)_{eff} = c_b\rho_b + c_p\rho_p\, h_p/h_b\,,$$

$$(\lambda)_{eff} = \lambda_b + \lambda\, h_p/h_b\,,$$

The heat capacities of the substrate $c_b\rho_b$ and powder layer $c_p\rho_p$ change according to law

$$c\rho = \begin{bmatrix} c_L\rho_L, T \ge T_m \\ c_s\rho_s, T < T_m \end{bmatrix} + L_m\rho_s\delta(T - T_m)\,.$$

In general case, the thermal conductivity coefficients also depend on temperature.

Analyzing the calculation results for $T(x,y,t)$, one can investigate the evolution of melting pool and heat affected zone, which has been determined using conditionally given temperature (for example, $T = 700 - 900$ K). If the temperature does not reach this value, the visible change in the material structure is not observed.

Certainly, this model is correct when the coating (or powder layer) is absent.

However, phase composition determined on the base of phase diagrams using temperature value found from pure thermal conductivity problem will be quite approximate. Correctness of the approach [16], where the results of thermal problem solution are used to determine the phase structure by the phase-field method is ambiguous from the methodological point of view.

Additional complexification of thermal models conditioned by the consideration of the temperature dependencies of the properties also leads to temperature change, variation of heat affected zone and melting pool shape. The results do not change qualitatively in three-dimensional problems. New capabilities appear for determination of the melting depth and temperature distribution along the third axis for massive parts.

Though, thermal-physical models can be efficient due to taking into consideration various kinetical phenomena, which lead to evolution of properties.

3. Formal kinetics of shrinkage

The formation of phases, porosity and evolution of defects, change of properties, shrinkage are kinetical processes. To take into account these processes while models are constructed, it is necessary to formulate the kinetical laws. Processes at micro- and meso-levels should be affected by kinetical parameters and kinetical functions.

For example, to ensure the required properties for preliminarily deposited powder coating, the additional thermal treatment is necessary that leads to densification and shrinkage of this layer. From physical point of view, the shrinkage is connected with melting and mass transfer in different phases, with adhesive forces appearance between individual particles etc. All mentioned processes are thermally activated and proceed at micro- and meso-levels: in the volume of individual particles, in pores between particles, at the interfaces. We assume that the independent investigations were made for constructing kinetical law. As a result, we come to the kinetic equation

$$\frac{dh}{dt} = \varphi(\rho_p(T), h) = \varphi(\Theta(T), h),$$

where Θ is porosity.

The simplest form of the kinetic equation is

$$\frac{dh_p}{dt} = \begin{cases} -k_p\left(\frac{h_p}{h_{min}} - 1\right)^s exp\left(-\frac{E}{RT}\right), & h_p > h_{min}; \\ 0, & h_p > h_{min}, \end{cases} \qquad (4)$$

$$t = 0: \quad h_p = h_{p0}, \tag{5}$$

where h_{min} is the minimal thickness of the coating obtained from powder layer with apparent density ρ_{p0}; k_2 is the constant of shrinkage rate; E is shrinkage activation energy (its value is determined by the processes limiting the shrinkage at micro-level), s is index in the kinetic function (it can be a whole or fractional number, depends for example, on particle surface shape). All parameters can be found from experiment or on the base of special physico-mathematical models. Lattice Boltzmann Equation method is suitable here [14, 17].

In the simplified approximation, we believe that thickness of powder layer is inversely proportional to density ρ_p. Because $\rho_p = \rho_{Me}(1-\Theta)$, we can write

$$\Theta = 1 - (1-\Theta_0) h_{p0} / h_p ,$$

where Θ_0 is the porosity of poured powder layer of thickness h_{p0}.

To demonstrate the additional possibilities appearing in the model, taking into account the shrinkage, we assume that the substrate is made from iron ($c_{bs} = 0.825, c_{bL} = 0.608$ J/(g·K), $\rho_{bs} = 7.61$, $\rho_{bL} = 7.87$ g/cm^3, $\lambda_b = 0.45$ J/(cm·sec·K), $T_{bm} = 1810$ K, $L_{bm} = 247$ J/g; $h_b = 0.5$ cm). The powder layer has the initial thickness of $h_p(t=0) = h_{p0} = 0.01$ cm and the following properties: $\lambda_p = 0.08$ J/(cm·sec·K), $c_{bs} = c_{bL} = 1.25$ J/(g·K), $\rho_{ps} = \rho_{pL} = 3.75$ g/cm^3, $T_{pm} = 2318$ K, $L_{pm} = 389$ J/g.

Model will allow describing, in a first approximation, the surface relief change due to shrinkage during surface treatment [15].

We assume that $H_x = 4.0$; $H_y = 3.0$ cm, and properties are assumed constant (except heat capacities near the melting temperatures).

Kinetic parameters ($E = 100$ J/mol, $h_{min} = 0.005$ cm, $k_p = 5 \cdot 10^2$ cm/sec) were chosen to illustrate the shrinkage. Shrinkage observed experimentally can be 30-40%.

For $q_0 = 1 \cdot 10^5$ J/(cm^2·sec) and for $V = 1{,}0$ cm/sec we get the following picture.

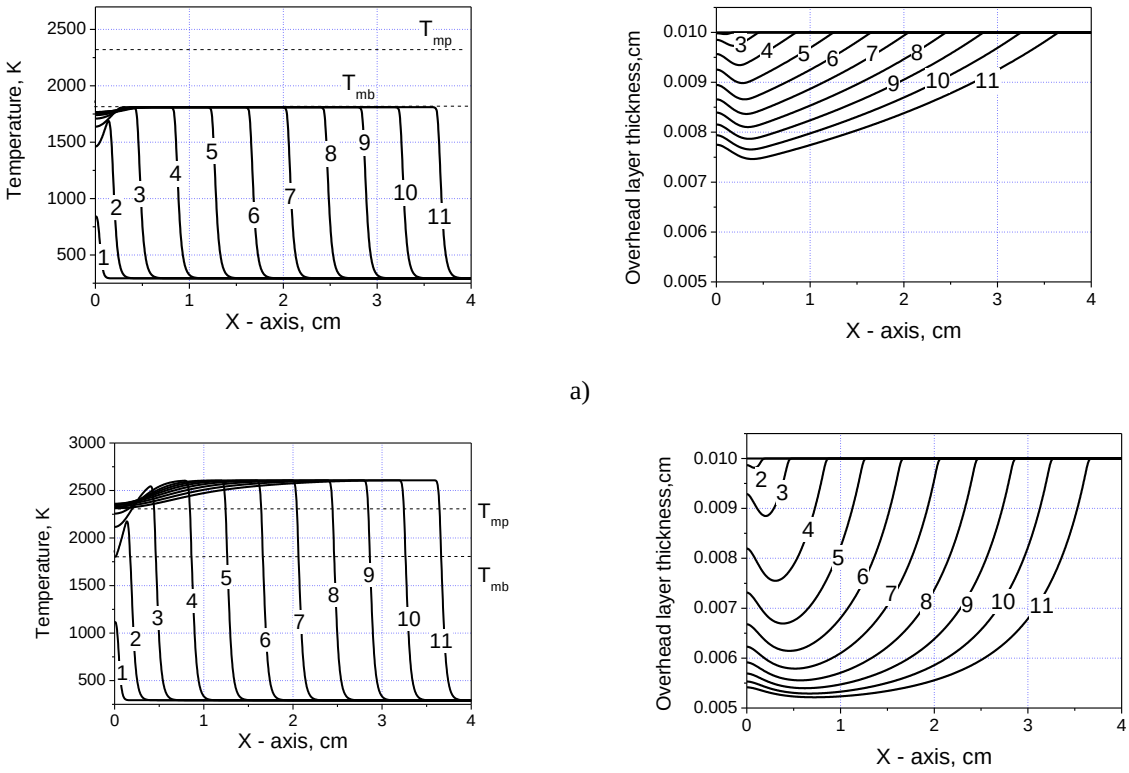
First, temperature in the heated zone does not reach melting temperature for powder layer (Figure 2a, left picture), but a small shrinkage takes place (Figure 2a, right picture). Even for quasi-stationary process (when maximal temperature does not change), the thickness of powder layer changes nonuniformly. If the temperature cycles at the points near the surface are different (Figure 3a), so in other points the temperature cycles are the same for different points along the X-axis. However, the shape of heat affected zone and of the area with temperature higher then T_{bm} change in time during the treatment. The pictures of the first line in Figure 4 illustrate this. The second line in the figures gives information about surface relief evolution during treatment.

If $q_0 = 1.5 \cdot 10^5$ J/(cm^2·sec) and $V = 1.0$ cm/sec, we obtain other results. Maximal temperature during treatment is higher than in previous case (Figure 2b), more substantial shrinkage is observed. This is shown in Figures 2 and 4.

Temperature changes similarly with time. However, we can see here the temperature slope connected with substrate melting more clearly (Figure 3b). When temperature exceeds the melting temperature of powder material, we can see the molten pool in addition to the heat affected zone. Isolines in Figure 4 (a and c) correspond to temperature 350, 700, 1800 and 2300 K.

Calculations show that the relief of the coating after treatment depends on all technological parameter and on the initial thickness of the powder layer.

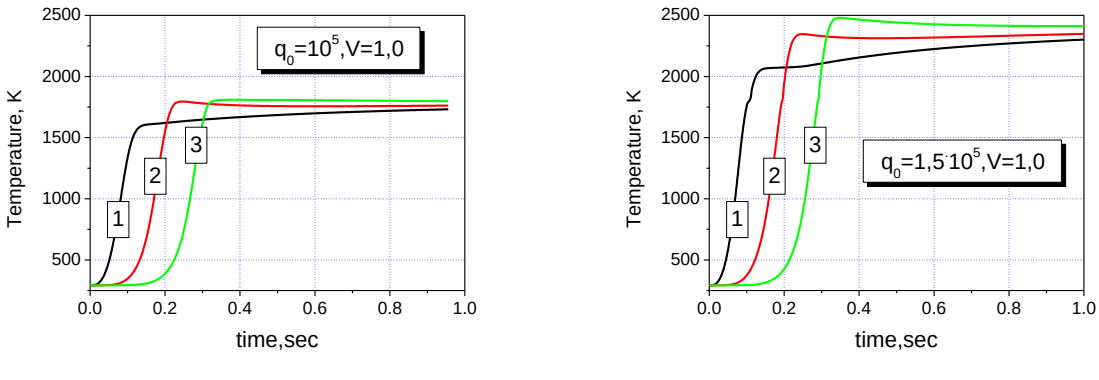
For practical applications, this model can be used to elaborate the recommendations for suitable parameter selection. By varying the treatment velocity, electron beam power, scanning thickness, etc., one can obtain enough uniform surfaces that ensure uniform properties.



a)

b)

Figure 2. Temperature and coating thickness along X-axis.
a) $q_0 = 1 \cdot 10^5$ J/(cm^2·sec); b) $q_0 = 1.5 \cdot 10^5$ J/(cm^2·sec)



a) b)

Figure 3. Temperature in time for three points along X-axis: 1) $x = 0.1$; 2) $x = 0.2$; 3) $x = 0.3$ cm

4. Conclusions

The results demonstrate that thermal-kinetic model qualitatively describes the observed regularities: temperature growth with effective flux density increase, source velocity reduction, thickness change during shrinkage. This allows predicting the thickness change during treatment after kinetical parameter identification. Richer opportunities appear when chemical reactions have been taken into account. Some examples are presented in [11, 15].

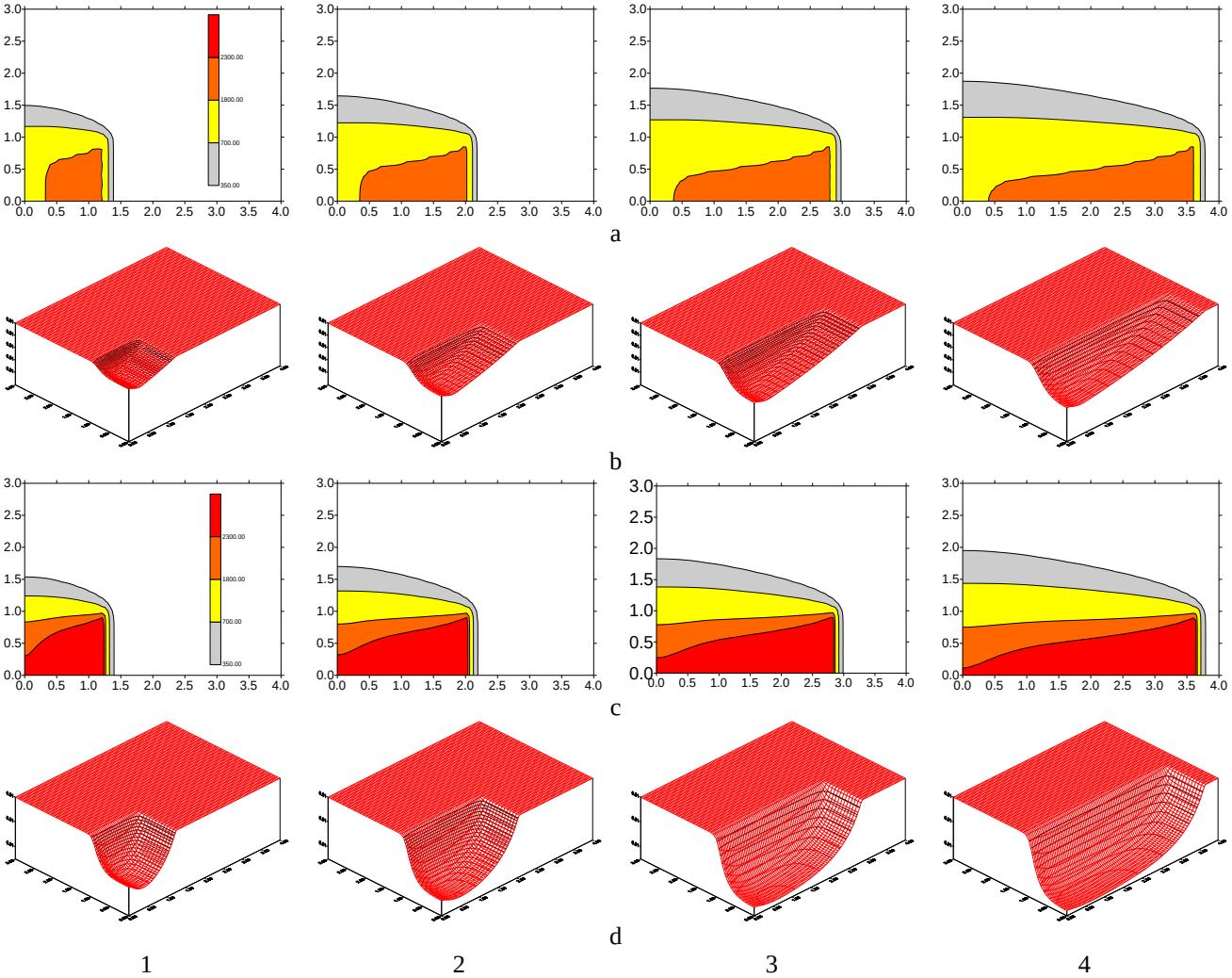


Figure 4. Evolution of temperature field (a, c) and thickness of powder layer (b, d) in time for $q_0 = 1 \cdot 10^5$ J/(cm^2·sec) (a and b) and $q_0 = 1.5 \cdot 10^5$ J/(cm^2·sec) (c and d).
$t =$ 1) 1.25 sec; 2) 2.05 sec; 3) 2.85 sec; 4) 3.65 sec.

Acknowledgments
This work was supported by the Ministry of Science and Education of the RF, project No. 11.815.2014/K.

References

[1] Herderick E 2011 Additive Manufacturing of Metals: A Review *J. Materials Science and Technology Conf. and Exhibition (MS&T 11) (16-20 October 2011 Columbus, Ohio, USA)* vol 2 pp 1413-25
[2] Poate J M, Foti G and Jacobson D C 1983 *Surface Modification and Alloying: by Laser, Ion, and Electron Beams* (New York: Plenum Press) p 414 (DOI 10.1007/978-1-4613-3733-1)

[3] Shipko A A, Pobol I L and Urban I G 1995 *Strengthening of steels and alloys using electron-beam heating* (in Russian) (Minsk: Nauka i technika) p 280
[4] Gong X, Anderson T and Chou K 2014 *Manufacturing Rev*. 2 **1** 1–12
[5] Thomas M, Baxter G J, Todd I 2016 *Acta Materialia* **108** 26 - 35
[6] Rykalin N N, Zuev A A and Uglov A A 1978 *The foundation of electron-beam treatment of materials* (in Russian) (Moscow: Mashinostroenie) 239 p.
[7] Sercombe T B and Hopkinson N 2006 *Advanced engineering materials* 4 **8** 260–4
[8] Ranogajec J, Djuric M, Radeka M and Jovanic P 2000 *Ceramics − Silikáty* 2 **44** 71–7
[9] Ade M and Haußelt J 2003 *Journal of the European Ceramic Society* **23** 1979–86
[10] Dai K and Shaw L 2005 *Acta Materialia* 18 **53** 4743–54
[11] Knyazeva A G, Pobol I L Gordienko A I., Demidov V N, Kryukova O N and Oleschuk I G 2007 *Physical mesomechanics* 3-4 **10** 207-20
[12] Knyazeva A G and Bookrina N V 2003 *Proc. of 12th Int. Conf. on radiation physics and chemistry of inorganic materials (23-27 September Tomsk, Russia)* pp 167-70
[13] Sahoo S and Chou K 2016 *Additive manufacturing* **9** 14-24
[14] Attar E and Korner C 2009 *J. of Colloid and Interface Science* **335** 84-93
[15] Knyazeva A G 2009 *Mathematical modeling of the systems and processes. Special issue of Vestnik PerGTU* (in Russian) **17** 66 – 84
[16] Krivilyov M D, Kharanzhevskii E V, Lebedev V G, Danilov D A, Danilova E V and Galenko P K 2013 *The Physics of Metals and Metallography* 10 **114** 799-820
[17] Gürtler F-J, Karg M, Dobler M, Kohl S, Tzivilsky I and Schmidt M 2014 *Proc.* of *Int. Solid Freeform Fabrication (SFF) Symp. - An Additive Manufacturing Conf. (4-6 August Austin, Texas, USA)* pp 1099-117