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Numerical investigation of the thermal transformation of composition powder particles in the technology of selective laser melting

V I Bogdanovich and M G Giorbelidze
Samara National Research University, 34, Moskovskoe Highway, Samara, 443086, Russian Federation

E-mail: bogdanovich@ssau.ru; m.giorbelidze@ssau.ru

Abstract. The results of mathematical model development for evaluation of thermal state of spherical particles of powder composition equally treated in the technology of selective laser melting are presented. This model considers: features of laser irradiation energy transfer to the particles having smaller size but comparable with the size of radiation spot diameter; energy transfer through the sphere upper half; material melting in the solidus and liquidus range; possibility of surface material evaporation and dependence of material thermophysical parameters on temperature. This model is adapted to be used in standard finite-element software ANSYS Transient Thermal that has been applied for numerical simulation using powder of heat-resistant nickel-chromium alloy. Process regularities have been discovered, and it was shown that the range value of particles size scatter of powder composition fraction used determines principle possibility of choosing laser treatment mode to provide high quality material after melting.

1. Introduction

Today new technological state of modern industry is realized due to both powerful computer-aided design systems and new technologies. Additive technology of selective laser melting (SLM) of powder materials is among them.

One of the main issues of SLM technology is reasonable choice of laser treatment mode of powder composition used. Significant amount of papers dealt with this issue [1-24], and they can be divided into two groups: papers based on experimental research results [7, 8, 10-14, 16-17] and papers based on mathematical simulations [1-6, 9, 15].

In the papers dealing with mathematical simulation, we can distinguish two levels of process – macro-scale and micro-scale. At the macro-scale level, powder layer is simulated as a solid material with effective values of physical-mechanical characteristics. The tasks of prediction of its heating and melting, thermal and residual stresses, material shrinkage and layer dimension variations are solved. At the micro-scale level, material is considered as a powder layer having various thickness and various arrangement of particles. The tasks of determining of thermal particles state, material spreading, estimation of penetration of melt into the lower layers, initiation and extinction of material voids are solved.

In papers dealing with mathematical simulation, researchers come to conclusion that the mode range of laser treatment is very narrow, and it requires considerable numerical and experimental researches to get the material of required quality.

Analysis of papers shows that potential material characteristics produced from powder under its layer-by-layer treatment are defined by the treatment mode of each separate particle of this layer. Further layer treatment by multidirectional travelling of the laser beam, thermal treatment or impregnation allows, if possible, enhancing these characteristics and leveling some negative consequences of local laser treatment of the powder layer.

The treatment mode of each separate particle is to provide at least its mandatory melting at the points of contact with other particles and the underlayer to provide topochemical interaction reactions of materials at these contact surfaces. However, under thermal flow density used and insertion of radiation through the upper half of the surface, particles of different sizes are heated up to various temperatures with substantial gradient throughout the height of their sections. This can result in heating of particles of other sizes less than melting point in the lower part and heating up to the vaporization temperature at the upper surface, but the heating temperature is optimum, if the particles are of the same size. For example, this different heating of particles of various sizes treated at the same mode allows us to conclude on insufficient informativeness of just experimental results and suggest a hypothesis on necessary use of particles just with certain scatter range of its sizes.

As applied to the tasks of mathematical simulation of thermal processes in powder composition particles, treated at the same mode of SLM technology, it is required to take into account surface evaporation, dissymmetry of laser irradiation through the particle upper surface and dependence of thermal flow absorption on its incidence angle.

Purpose of this paper is to report research results got during development of proper mathematical model of evaluation of thermal state of particles of powder composition treated at the same mode in the technology of selective laser melting and adapted to be used in the standard software ANSYS Transient Thermal. This mathematical model suits for applied use to determine optimum mode of composition treatment. Some results of numerical research of powder composition of heat-resistant nickel-chromium alloy ВВ751П are given.

2. Process conceptual model

In the typical SLM process, powder is put on the platform surface to manufacture a workpiece or it is put on the previously alloyed layer with successive vertical shift of the movable platform part by 30…100 μm. Powder is levelled by height and consolidated with the scraper travel that is pressed to the fixed part of the platform surface. Powder layer is treated by the laser energy beam continuously travelling the desired path along the model section contour in order to fuse the powder at this contour. Then powder fusion within the distinguished contour is carried out when the beam is traveling along the desired continuous path. At the completion stage, the layer is blown by a laminar gas flow to remove air-floated particles.

3. Mathematical modeling of particle heating in selective laser melting

Statement of mathematical model of the processes of heating, melting, the following crystallizing and cooling-down of the spherical particle of the metal alloy with the temperature range of the phase transition is to include corresponding differential heat conduction equation, initial and boundary conditions. Boundary condition is to consider features of heat transfer to the particle from laser irradiation and features of heat exchange between the particle and the environment.

It can be shown that typical differential heat conduction equation for an isotropic body with emitting and absorbing heat in the volume [19] can be brought to the following form considering phase material transformation at the solidus and liquidus range, possibility of surface evaporation and adapted to end-to-end finite-element procedure to be used in the standard software ANSYS:

$$c_{ef}\left(T\right)\rho\left(T\right)\frac{\partial T}{\partial t}=div\left[\lambda\left(T\right)grad\left(T\right)\right] \qquad (1)$$

The following designations are used in (1):

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$$c_{ef}\left(T\right)=c\left(T\right)+\frac{L}{T_L-T_S}\varphi\left(\frac{T-T_S}{T_L-T_S}\right)\left[\eta\left(\frac{T-T_S}{T_S}\right)-\eta\left(\frac{T-T_L}{T_L}\right)\right]+\frac{L_{ev}}{T_{ev}}\delta\left(\frac{T-T_{ev}}{T_{ev}}\right), \tag{2}$$

where $T\left(t,\vec{r}\right)$ is temperature at the time moment t of the body point having coordinate $\vec{r}$; $c\left(T\right)$, $\rho\left(T\right)$ and $\lambda\left(T\right)$ is specific thermal capacity, density and material thermal conductivity coefficient; T_S, T_L and T_{ev} is solidus and liquidus temperature and material evaporation temperature; L and L_{ev} is specific fusion and evaporation heat; div and $grad$ is differential operators of divergence and gradient; $\eta\left(u\right)$ is unit Heaviside function ($\eta\left(u\right)=0$ when $u<0$ and $\eta\left(u\right)=1$ when $u\geq 0$) and $\delta\left(u\right)$ is Dirac delta function with corresponding dimensionless arguments; $\varphi\left[\left(T-T_S\right)/\left(T_L-T\right)_S\right]$ is rate function of phase transition (in the instant melting case it is called by analogy with the known function called crystallization rate [20]) connected with specific volume share of new liquid phase in the nominal volume of melted material in the liquid crystal area of the phase transition $\psi\left[\left(T-T_S\right)/\left(T_L-T\right)_S\right]$ by the relation $\varphi\left(u\right)=d\psi(u)/du$.

This differential heat conduction equation (1) retains the same in different body parts with and without phase transitions as well as for various stages of its heating and cooling.

Initial condition is the equality of the temperature to the initial temperature of the sphere material at the time moment $t=0$:

$$T\left(0,\vec{r}\right)=T_0\left(\vec{r}\right). \tag{3}$$

Boundary condition is determined by the fact that laser irradiation striking the upper sphere surface is converted into the thermal flow inserting the sphere surface normally to the upper half sphere material. It acts during the period of passing over the particle. Boundary condition is also determined by convection cooling and thermal radiation of the whole surface. In a spherical coordinate system that is convenient in case of temperature distribution in the spherical particle, boundary condition is the following:

$$\lambda(T)\frac{\partial T}{\partial r}=q\left(t,\theta,\varphi\right)\left[\eta\left(\theta\right)-\eta\left(\theta-0.5\pi\right)\right]-\alpha\left[T-T_c\right]-\varepsilon\sigma\left[T^4-T_c^4\right],\text{ when } r=R. \tag{4}$$

The following designations are used in (4): R is spherical particle radius; α is coefficient of convective heat exchange; ε is integral radiation coefficient of the sphere surface; σ is Stefan-Boltzmann constant; T_c is gas temperature in the chamber; θ and φ is zenith and azimuth angles of the spherical coordinate system connected with sphere center; difference of unit Heaviside functions taking into account the fact that thermal flow to the sphere surface does not equal zero only in the zenith angle area $0\leq\theta\leq 0.5\pi$ is given in square brackets.

Thermal flow value $q\left(t,\theta,\varphi\right)$ in general case is to depend on time *t*, zenith θ and azimuth angle φ of spherical coordinate system as laser irradiation source travels over the sphere with constant speed v. In addition, thermal flow density is also to depend on zenith θ as material absorption coefficient depends on incidence angle of laser irradiation. Therefore, temperature in the spherically symmetrical ball depends on the position of laser spot over the sphere, and it is not symmetrical of zenith and azimuth angle.

In this formulation boundary problem (1) – (4), if $q\left(t,\theta,\varphi\right)$, it can be solved with numerical simulation using standard software ANSYS. Results of this numerical simulation have shown that calculations are very computer time-consuming, but the result is complex to analyze and insufficiently informative to develop technological suggestions on choice of optimum treatment modes of powder composition with sizes scatter range.

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4. Results and discussion

Numerical simulation of particle heating process introduced as a boundary problem (1-3) has been carried out using standard software ANSYS. Heating mode of the powder composition has been at heat flux q_0 at source traveling speed v. Adequacy of the mathematical model has been verified and confirmed by means of model parameters of the material based on accuracy of numerical calculations in comparison with results of known exact and approximate analytical solutions. It is also based on estimation of stability and convergence of solutions under decreasing of partition interval sizes, on calculation error of relation (4), and on comparison with the results of special experimental research.

Composition treatment mode has been chosen by the following way. According to the particle heating simulation with particles of maximum diameter in the composition (for example, maximum diameter 50 or 40 μm) when the temperature in the sphere bottom point reaches material liquidus temperature ($T_L = 1346$ °C), and the temperature in the sphere top point does not exceed material evaporation temperature ($T_{ev} = 2913$ °C) heating time of the particle has been chosen. According to this time, value of source travel speed has been determined, and heating period and heat flux that are to be applied to the particles of other diameters when treated at the same mode.

Typical results of mathematical simulation are shown in Figure 1 and Figure 2.

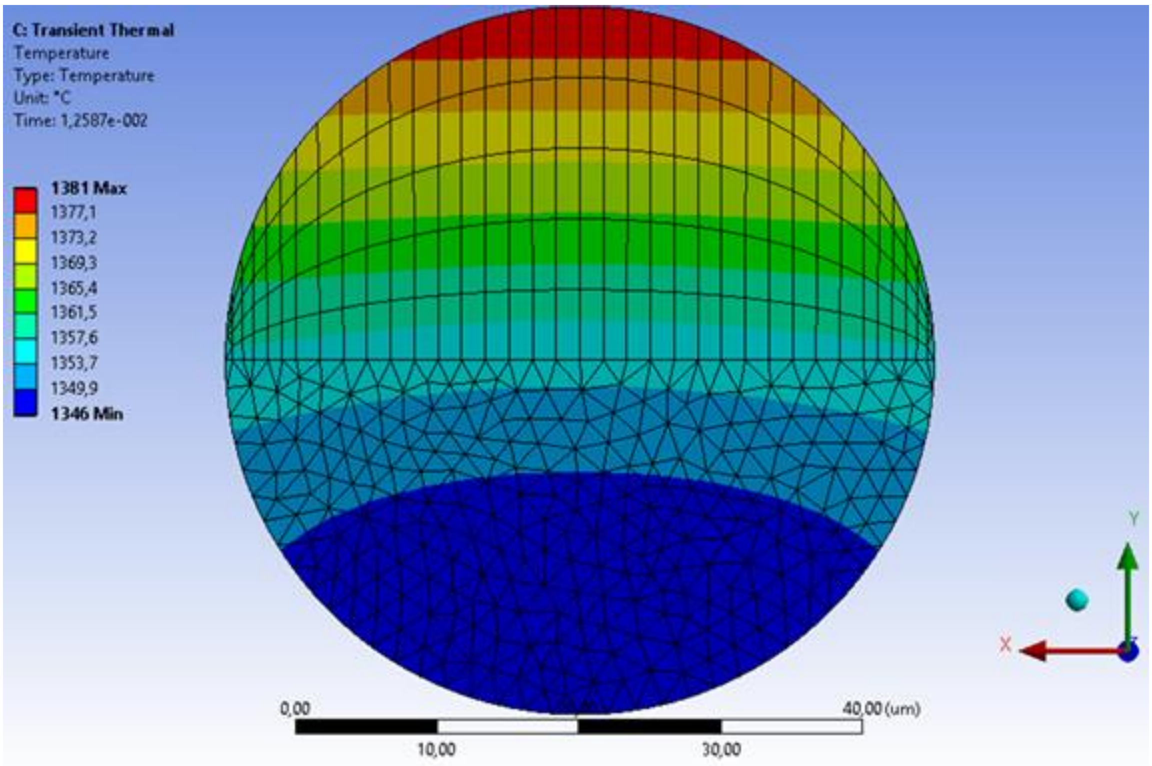

Figure 1. Temperature distribution of the sphere cross-section with diameter 50 μm when heat flux $q_0 = 1 \cdot 10^8$ W/m^2 at the time moment 0.012587 s when its temperature at the bottom point has reached liquidus temperature 1346 °C.

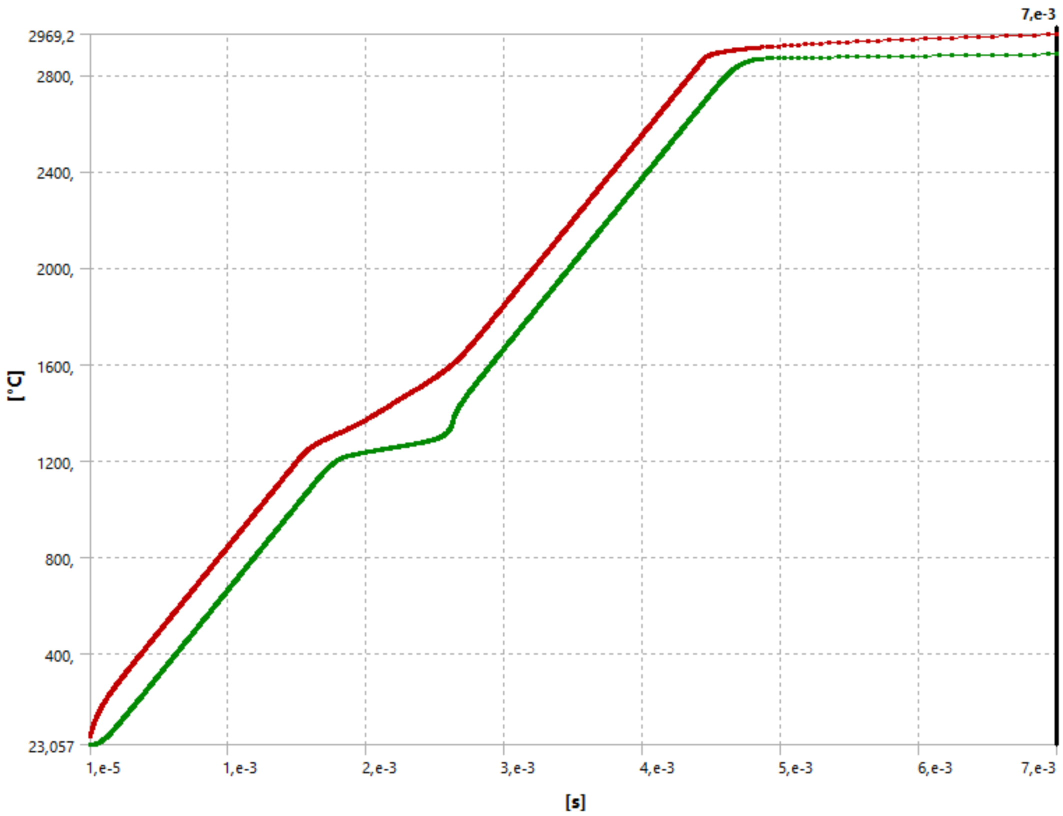

Figure 2. Temperature of the top and bottom points of the sphere with diameter 50 μm depending on the time period at heat flux $q_0 = 1 \cdot 10^8$ W/m^2.

5. Conclusion

It has been found out that for the powder composition with particle diameters 50…20 μm there is no treatment mode at which the particles with maximum diameter 50 μm are completely melted, and the particles with minimum diameter 20 μm do not reach boiling at intensive evaporation. As a result, some research has been carried out to choose treatment mode of powder composition with narrower particle scatter range within 40…20 μm that has shown availability of the mode with complete melting of all the particles and just since evaporation of the particles with 20 μm diameter.

As a result of numerical simulation SLM, basic treatment mode of powder composition 40…20 μm has been recommended. It provides heat flux $1.206 \cdot 10^9$ W/m^2 and travel speed of the laser spot 328 mm/s. Preliminary sizing of powder in delivery condition with extraction of recommended fraction is suggested.

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