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Numerical simulation of heat transfer and melting of Fe-based powders in SLM processing

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Abstract. Modelling of selective laser melting (SLM) of Fe and stainless steel powders has been performed to analyze unsteady heat transfer in a porous medium under conditions of rapid phase transformations. The pulsed laser heat source develops high temperature gradients that lead to large solidification velocities, which can be used in acquisition of complex microstructures in SLM manufacturing. First, the effective thermal conductivity as a function of the local porosity which is a dynamically varying parameter in SLM was evaluated numerically. It showed a high role of heat transfer through the gas phase in powders with low thermal conductivity, i.e. in stainless steel. At the porosity 65% and above, the mechanism of heat transfer drastically changed and a linear dependence of thermal conductivity on porosity frequently used in literature becomes incorrect. Second, the obtained dependence was accounted for modelling of thermal fields and powder consolidation in the powder bed. The results of simulation agree well with the obtained experimental data and show the importance of correct dynamical evaluation of the thermophysical properties in SLM processes.

1. Introduction

Selective laser melting of metallic powders is a complex process. Therefore its computer simulation is important in modern material sciences and technology. Selective laser sintering (SLS) and melting (SLM) are the successfully developed techniques which allow us to modify phase and structural characteristics in a thin surface layer [1, 2] located on the substrate or formerly processed powder layers. Extension of this method towards processing of ultrafine powders through pulsed laser annealing was done for roughness reduction of SLM produced parts [2, 3]. The key feature of pulsed laser powder annealing is enermous local heating of the surface and large thermal gradients and velocities during the treatment. Due to high velocities of the solidification fronts, melting and crystallization of ultrafine (submicron and nanoscale) particles proceed under highly nonequilibrium conditions. Several literature sources estimate the cooling rates of the melting pool during the laser processing as very high [4, 5]. Both sintering and remelting process of ultrafine powders could be used as the suitable techniques for synthesis of metastable metallic materials [6] with desired phase composition. A characteristic time of the cycle "heating-melting-solidification" or "heating-sintering" depends on the annealing mode and follows from the processing parameters. In pulsed lasers which may lead to high melting/solidification velocity, the duration of a single impulse is about $\tau \sim 10^{-6} \div 10^{-3}$ s. Hence, in such short times it is difficult to control the dynamics of the remelting process and proper selection of the optimal processing parameters is vital. The objective of this study is the development of a comprehensive model and then verification analysis of laser sintering and

melting process of ultrafine powders. In the paper, the results of experimental and computational examination are used to reveal the effect of dynamic thermal properties of the powder media under high energy pulsed laser treatment on the dynamics of melting and solidification during SLM processing.

Transport of heat through a porous medium is of great interest in relation with its regular and stochastic properties since in SLM the effective thermal properties control the dynamics of melting and solidification [5, 7]. The structure of a porous media is complex and irregular and it is defined by a wide distribution of morphology and size of pores [8]. Due to the fact that powder in SLM is spheroidized, the simplest approximation of particles by spheres can be used. However, this approximation somehow simplifies the results of analysis for real industrial systems [9]. Thus, the detailed prediction of the effective thermal conductivity of heterogeneous media requires consideration of the shape and size distribution, conductivity of each particle, atmosphere and heat exchange between the metal and gas phases [10]. Calculation of the effective heat conductivity for a case of stochastic filling of the powder can be made by combination of the classic packed bed modelling [8, 10] and the stochastic random filling model [9]. This approach is presented in this article.

The computing of SLM processing considering the whole powder layer including such effects as compacting and remelting of powder under the high-energy laser irradiation is represented by a wide range of models [2, 5, 7]. They all can be reduced to three classes in description of laser processing: (i) models of the arbitrary powder bed that directly account for partial melting and mass transfer coupled to heat conduction (implemented by the finite volume method); (ii) models with the stochastic distribution of particles which incorporate the phase state of the system using a state functions to determine the molten domain (by the discrete element or cellular automata methods); (iii) models which consider the powder in the approximation of a continuous medium assuming shrinkage of the powder as a continuous function (by the finite element method, models with a moving boundary).

In our work, the approximation of a continuous medium is used for modelling of heating of the powder bed, sintering and consolidation [11, 12, 13] during SLM of iron and stainless steel (CL20ES) powder by the pulsed infrared optic fiber YAG:Nd^{3+} laser. To control the effective thermal conductivity k_{eff} a state function $k_{eff}(\varepsilon)$ is used where ε is the local porosity. The function $k_{eff}(\varepsilon)$ is calculated separately for Fe and stainless steel powders under different atmosphere conditions (Vac, Air, Argon) suitable for SLM manufacturing.

2. Computer simulation of local heat transfer in the powder bed

In our work, we directly model heat transfer in the metallic powder beds using stochastic filling of the representative volume with a number (up to 10^3) particles. The numerical model gives us a possibility to calculate the dynamics of heat propagation in a metal powder with the given porosity ε treated in inert atmosphere or in vacuum. The model is allowing the variation of the fractional composition of particles, their size distribution and relative density of the bed.

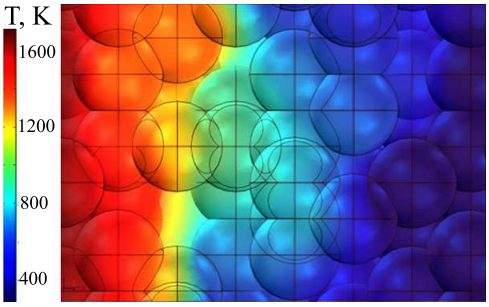

Figure 1. Instantaneous thermal field T in the ultrafine Fe powder bed calculated for the particles with a radius R_p=1.5 μm in argon and the porosity $\varepsilon = 0.65$. The time is $t = 3 \cdot 10^{-5}$ s and the evaluated effective heat conductivity for this case is $k_{eff} = 3$ W/(m · K).

2.1. Model

The powder bed was modelled by random placement of spherical particles according to the size and contact positions verified by scanned electron microscopy. The average radius of the particles in ultrafine iron powder was found about $R_p = 1.5$ μm and for stainless steel $R = 45$ μm assuming Gauss-type size distribution [1, 5, 14]. The specified porosity is achieved by removal of random particles from the bed till the target average density (or porosity ε) is attained. The spheres intersect each other by $10 - 20\%$ of the radius R_p to model heat contacts through each pair of particles.

For construction of a mixed two-phase system "gas-metal", the transient heat conduction equation is used. The two-phase problem with heat sources/sinks was solved using the finite element method. There is no need to take into consideration the effect of heat irradiation in the system of particles because of its small contribution to the overall energy balance. The convection mechanism of heat exchange was also neglected for the specified capillary systems [9] due to a pulse mode of processing ($\tau = 10^{-3}$ s for the used laser system). Thus, the time scale of heat annealing of the powder was significantly shorter than a characteristic time of effective gas flows through the powder. Then the boundary value problem for heat conduction in the powder bed is

$$C_p^{\text{gas}}\rho^{\text{gas}}\frac{\partial T}{\partial t} = k^{\text{gas}}\nabla^2 T, \quad C_p^{\text{metal}}\rho^{\text{metal}}\frac{\partial T}{\partial t} = k^{\text{metal}}\nabla^2 T, \tag{1}$$

$$T|_{t=0} = T_{amb}, \quad T|_{z=0} = T_m, \quad \mathbf{n}\cdot k\nabla T = 0 \text{ at other boundaries}, \tag{2}$$

where C_p is the specific heat capacity, ρ is density, k is the thermal conductivity for each phase. For the interphases between gas and metal a continuity of heat flows and temperatures was defined. The temperature at the boundary $z = 0$ was selected as the melting temperature $T_m^{\text{Fe}} = 1808$ K and $T_m^{\text{stainless steel}} = 1713$ K. In Figure 1 the instantaneous thermal field calculated in the powder bed is presented.

2.2. Evaluation of the effective thermal conductivity

The inverse problem of heat conduction [15, 16] was solved in the self-similar approximation which was used to get the effective thermal diffusivity coefficient α_{eff} as follows

$$\frac{\partial T}{\partial t} = \alpha_{eff}\nabla^2 T, \quad \text{which leads to a solution} \quad T(z,t) = T_m - (T_m - T_{amb})\,\text{erfc}\left(\frac{z}{\sqrt{4\alpha_{eff}\,t}}\right). \tag{3}$$

In performed simulations, we take a number of numerically calculated profiles at fixed times in the mixed gas-metal domain. Then a minimization Levenberg-Marquardt procedure to the functional $T^{\text{num}} - T^{\text{analyt}}$ was applied. Figure 2 depicts both the calculated temperature probes at different locations of the domain and the fitted semi-similar solution. In this manner the effective diffusivity coefficient for the specific times can be approximated. Then α_{eff} is averaged in time and the effective thermal conductivity for the two-phase powder is obtained by

$$k_{eff}(\varepsilon) = \alpha_{eff}\left(C_p^{\text{gas}}\cdot\rho^{\text{gas}}\,\varepsilon + C_p^{\text{metal}}\cdot\rho^{\text{metal}}\,(1-\varepsilon)\right) \tag{4}$$

for each set of heat profiles for given ε. Since this task is devoted to evaluation of the effective thermal conductivity as a function of geometric characteristics of powder, the heat capacity C_p of both gas and metal is here assumed to be temperature independent. Dependence of k_{eff} on temperature is introduced in the model below where the macroscopic model of sintering/melting is considered.

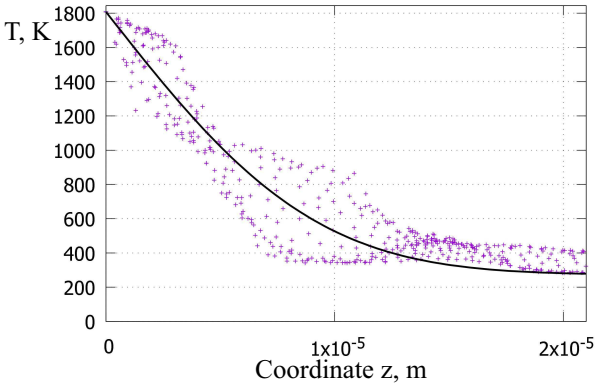

Figure 2. Temperature field (denoted by the color dots) calculated numerically for Fe powder in air with the porosity $\varepsilon = 0.65\,(65\%)$ at time $t = 10^{-5}$ s. Propagation of a heat wave experiences thermal resistance on gas inclusions which leads to deterioration in effective heat transfer. The black line is the approximated curve plotted for the self-similar solution (Eq. 3). The obtained effective thermal diffusivity is $\alpha_{eff} = 2.265 \cdot 10^{-6}$ m^2/s compared to the $\alpha_{\mathrm{Fe}} = 2.85 \cdot 10^{-6}$ m^2/s.

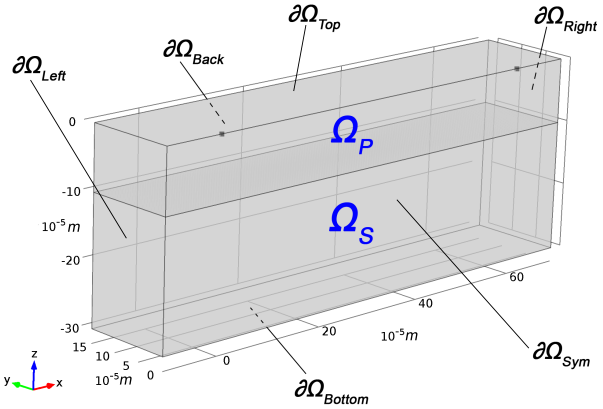

Figure 3. Computational domain for simulation of the powder bed melting. The top subdomain corresponds to the powder bed with a height of $h_0 = 100 \div 150$ μm. The bottom subdomain represents the stainless substrate. In SLM the previously processed layer acts as the substrate. The finite element mesh contains up to 10^7 degrees of freedom.

3. Simulation of sintering and melting of the powder bed

Mathematical description of underlying in SLM thermophysical phenomena [12, 13] is provided by the heat conduction equation adapted for enthalpy of phase transitions [15, 16, 17] and a surface heat source F due to laser annealing. Two conjugated variables temperature T and specific enthalpy H of the metal fraction are used, Eqs. (5) and (6). In addition, Eq. (7) [18] for the kinetics of local porosity ε is assumed. Then the given system of equations is as follows:

$$\frac{\partial T}{\partial t} = \frac{\partial T}{\partial H}\frac{\partial H}{\partial t}, \tag{5}$$

$$\frac{\partial H}{\partial t}(1-\varepsilon) = \nabla \cdot (k_{eff}(\varepsilon)\nabla T) + F, \tag{6}$$

$$\left.\frac{\partial \varepsilon}{\partial t}\right|_{\Omega_P} = -\varepsilon A \exp\left(\frac{E_a}{RT}\right), \tag{7}$$

$$\Delta Z|_{\Omega_P} = \frac{h_0(1-\varepsilon)}{1 - \int_z \varepsilon dz/h_0} - h_0, \tag{8}$$

where Ω_P is the powder subdomain (Fig. 3), A is the exponential factor describing the dynamics of consolidation of the powder, E_a is the energy of activation of viscous flow of liquid metal. The displacement ΔZ along the z axis defines an actual position of the top boundary according to local consolidation of the powder. Its definition includes the initial thickness h_0 of the powder layer and the integral on local porosity ε along z-direction in the powder. The effective conductivity $k_{eff}(\varepsilon)$ given in Eq. (6) represents a correlation between the thermal

conductivity and local structure of the powder bed. Equation (7) is the Arrhenius-type [18] kinetic equation which is often used for description of viscoplastic flow in multiphase systems with phase transitions. In our model it is used for description of the dynamics of the powder porosity [12]. Equation (8) defines the unsteady position of the top boundary $\partial\Omega_{Top}$ in time, Fig. 3. At $\partial\Omega_{Top}$, the boundary heat source F is implied to reproduce laser heating of the surface conjugated to the convective and radiate cooling. The computer model has been implemented using the commercial software COMSOL Multiphysics (licence No. 1056903) in the weak form. The processing parameters [12, 13, 19] were selected for the laser facility BULAT LRS which was used for SLM processing.

4. Results and discussions

The dependence of the effective thermal conductivity on gas atmosphere is presented in Fig. 4. The calculated points are fitted by a polynomial function which depends on the local porosity ε. Then this function is included in the macroscopic model in which heating, melting and solidification of the powder bed are simulated in the approximation of a continuous medium. It allows us to account for the effect of dynamically changed porosity in powder consolidation.

The effect of gas atmosphere for powders with low conductivity like stainless steel was analyzed. In powders with relatively small porosity or in powders with relatively high thermal conductivity the presence of air or protective atmosphere in pores is insignificant. The influence of atmosphere can not be neglected if the initial porosity ε achieves a value 0.6. It happens due to the percolation effect in powders with high porosity $\varepsilon > 0.7$ where thermal contacts between particles are not sufficient. As a result, quality of the fabricated SLM parts can be controlled by reduction of the initial porosity by mechanical milling of the powder.

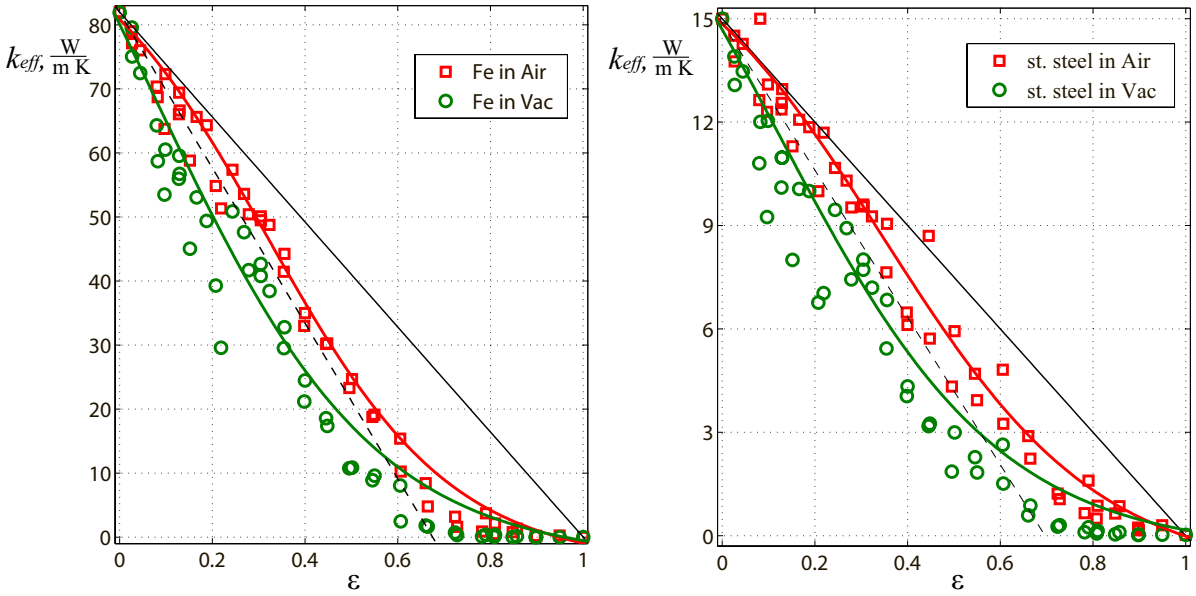

Figure 4. Dependence of the effective thermal conductivity k_{eff} on the local porosity ε calculated for a) Fe powder in vacuum (green curve and circles) and air (red curve and circles); b) stainless steel CL20ES powder in vacuum (green curve and circles) and air (red curve and circles). The dashed line represents the theoretical percolation limit for the medium, the black thin line represents the geometrical linear interpretation of the porosity.

A comparison of the calculated profiles in the melted powder with optical images taken

in similar full-scale experiments is given in Fig. 5. Introduction of the effective thermal characteristics such as the effective thermal conductivity $k_{eff}(\varepsilon)$ has made it possible to achieve good qualitative and quantitative agreement with the experiment [19].

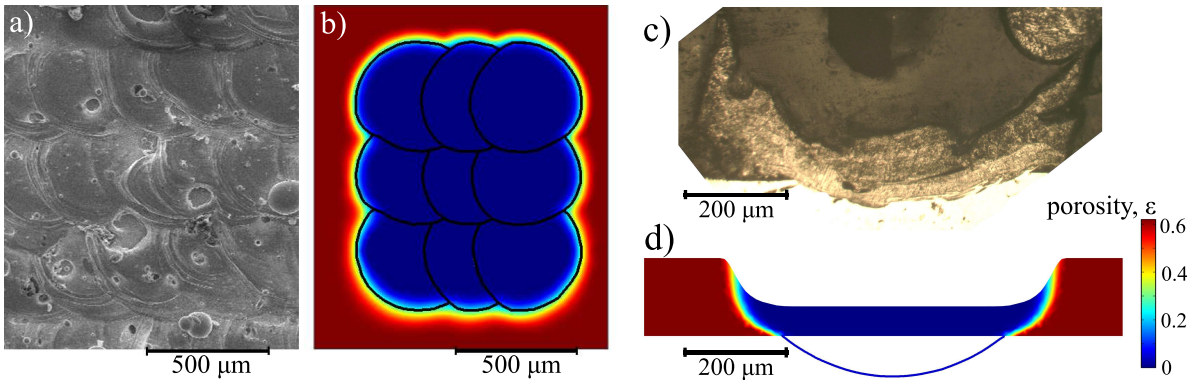

Figure 5. Comparison of the optical images (subfigures *a* and *c*) of the sample with the results of numerical simulation (subfigures *b* and *d*). Good quantitative agreement is achieved both in the track patterns and cross sections for Fe powder. The processing parameters for SLM of the stainless steel substrate were as follows. The frequency of the laser pulses is $\nu = 50$ Hz and the initial porosity is $\varepsilon = 0.6$. a,b) Top view of the melted powder layer, pulse energy is $E_{imp} = 3.4$ J, pulse duration $\tau = 1.5 \cdot 10^{-3}$ s. c,d) Cross sections, $E_{imp} = 2.2$ J, $\tau = 4 \cdot 10^{-3}$ s.

5. Conclusions

The effective thermal conductivity k_{eff} as a function of porosity ε for Fe and stainless steel powders were calculated in a series of computer simulations. The obtained relations can be used for modeling of powder consolidation in selective laser sintering/melting. It is also useful for estimation of the effect of porosity on partial melting.

The purpose of this work was the development of a mathematical model and study of melting and consolidation of the powder bed. In a series of computations, the underlying in SLM phenomena were analyzed for the industrially relevant Fe-based powders. Good agreement with the experiment data ensures that these data are useful for improvement of quality of the melted tracks. Further optimization of the whole process to receive the highest speed of fabrication at decent quality of the compacts and adhesion to the substrate was suggested.

6. References

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