Modelling Thermal Capillary Effects and Flow in the Molten Pool during Selective Laser Melting

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Abstract: Selective Laser Melting is a 3D printing technique very common for metals. It is designed to use a high power-density laser to melt powder and build parts layer-by-layer. Simulation of that process comprising a good number of phenomena, taking place at high temperature, has shown many challenges. In this work, simulation of melt flow, mainly due to thermal capillary effects in the molten pool during laser scanning, is done on 316 stainless steel material using finite element method with COMSOL Multiphysics software. It is demonstrated that the heat convection towards the boundary of the molten pool plays a key role in defining the size of the molten pool. This is a key parameter for prediction of the quality of printing.

Keywords: Selective laser melting, Marangoni effects, 316L stainless steel, thermal capillary effects.

Introduction

Laser additive manufacturing has become an interesting field of Material Engineering which is revolutionizing industrial processes. Selective Laser melting (SLM) is a widely used additive manufacturing technique for 3D printing of metal structures. This process has a particular complexity in modeling and simulation due to multiple phenomena taking place in a large range of temperature; from room temperature to thousands of degrees. Currently, different SLM models have been proposed. Some methods can be used for only a further understanding of the process. Others can even be used in an attempt to predict and optimize SLM process parameters for optimal printing. In the latter case, the size and geometry of the molten pool are the main information leading to knowing the quality and density of printed material. Temperature profile, temperature gradient and cooling curves are also useful information that can help in a qualitative prediction of the microstructure and solid phases in the printed material. However, in this modeling challenge, some researchers tend to use the most simplified way eliminating the fluid dynamics in the molten pool. In this work, we present a way to use COMSOL Multiphysics to model thermal capillary effects and

fluid flow inside the molten pool in a single scan or multiple scan model of SLM. The velocity field in the molten pool is simulated. The impact of neglecting the fluid dynamics in the molten pool can also be discussed.

Model Set-up

During SLM, a laser source follows a predesignated 3D CAD model to scan from top a layer of powder deposited on a bulk substrate. After consolidation process, the molten powder solidifies into a dense material which sticks on the existing printed substrate then the process is repeated through a layer-by-layer build-up of the whole printed material. Figure 1 shows an illustration of a multiple scan model set-up. However, to save computation time, in this paper we will consider a simple single scan to demonstrate the modeling techniques as seen in Figure 2. Referring to the experimental set-up commonly used in our research group, model parameters are given in Table 1. The material considered is 316L stainless steel. Thermal properties of the material are taken from [1] and plotted in Figure 3.



Figure 1. Illustration of the model set-up for SLM multiple scans. Traces of molten pools at different times are shown. The white contour corresponds to the molten pool at the actual time.

Parameter (Symbol)	Values [Unity]
Length (L)	1000[µm]
Width (W)	150[μm]
Height (H)	150[μm]
Powder layer Thickness (1)	60[µm]
Scanning speed (<i>v</i>)	750[mm/s]
Spot radius (<i>r</i>)	40[µm]
Surface emissivity (ε)	0.4
Laser power (P)	175[W]
Melting temperature (Tm)	1450+273[K]
Solidus Temperature (Ts)	1385+273 [K]
Powder porosity (Ø)	0.48
Latent heat of fusion (Lf)	260[J/g]
Dynamic viscosity	0.0028[kg/(m s)]
Temperature derivative of the	
surface tension	-0.04685[m N/(m K)]
Total absorptivity of powder bed (A)	0.63

Table 1. Model parameters

General modelling of SLM phenomena

Laser energy absorption during SLM is one of the most important physics in SLM modelling. When using Finite Element (FE) methods, the best way to model laser absorption in the powder bed would be using a volumetric heat source delivered from the Radiation Transfer Equation (RTE) for a powder layer deposited on top of a bulk substrate. That solution, which considers multiple reflections through air voids and diffractions, has shown a good agreement with the ray tracing method. For simplicity, in this work we adopt a simple volumetric energy deposition model in which we consider a penetration depth and power absorptivity of about the same values as those obtained using more appropriate models like RTE or RT [2], [3]. Volumetric power absorption intensity is given by (1):

$$Q = \frac{2AP}{\pi r^2 \delta} \exp\left\{\frac{2[(x-vt)^2 + y^2]}{r^2}\right\} \exp(\frac{-|z|}{\delta}).$$
 (1)

In the expression (1), A is the total absorptivity of the powder bed, P is the laser power, v the scanning speed, r the Gaussian laser spot radius, t the scanning time and δ the penetration depth.

Boundary conditions are treated using the "infinite element" feature of COMSOL Multiphysics[4]. In this concept, a small chunk of material studied is surrounded by an infinitely big material, which is a good approximation of the SLM situation.

In a general way, heat transfer can be described by the heat equation (2).

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p u. \nabla T - \nabla (k \nabla T) = Q \quad . \tag{2}$$

In (2), T is the temperature, ρ is the material density, c_p is the heat capacity and k is the thermal conductivity.

Two boundary conditions are defined on the top surface: the heat liberated by surface thermal radiation and the heat exchanged with the gaseous medium by convection as in equation (3):

$$k \left[\frac{\partial T}{\partial z} \right]_{z=H} = \varepsilon \sigma \left(T_o^4 - T^4(x, y, H, t) \right) + h(T_o - T(x, y, H, t)).$$
(3)

In expression (3), ε is surface emissivity, σ the Stefan–Boltzmann constant, T_o room temperature, H the height of the model geometry and h convective heat transfer coefficient.

Phase change was modeled using the apparent heat capacity model described in the "Heat transfer with phase change" feature of COMSOL Multiphysics [4]. Heat capacity and density of powder were approximated from those of bulk metal by linear combinations of properties of gas and bulk metal according to the porosity of the powder. Thermal conductivity of powder is model using the model of Sih and Barlow[5].

Thermal capillary effects and flow in the molten pool

During SLM, molten material is subjected to some fluidic forces that can cause considerable movement. The influence of the velocity field on the heat transport mechanism can be enormous. Most important phenomenon is the Marangoni effects, due to surface tension gradient, also called thermal capillary effects when this gradient is due to temperature difference. In FE numerical methods it can be modeled as a shear stress on the upper surface of the molten pool as in expression (4) where *s* denotes the molten pool top surface, $\frac{d\gamma}{dT}$ is the coefficient of the surface tension which is characteristic of a given material, γ is the surface tension and T_{ref} is a reference temperature which is taken to be the melting point.

$$F^{Marangoni} = \nabla_{s} \gamma , \quad \gamma = \gamma_{0} + \frac{d\gamma}{dT} \left(T - T_{ref} \right).$$
(4)

Due to high temperature gradient in the molten pool, a gradient in material density will be induced and causes a volume force in the molten pool given by (5):

$$F_g = g(\rho - \rho_{ref}) \,. \tag{5}$$

In expression (5), ρ_{ref} is reference density taken at temperature T_{ref} and ρ is the temperature-dependent material density. To be able to consider the flow in the molten pool, Navier-Stokes equations (6) were used to model the laminar flow in the molten pool.

$$\begin{cases} \rho \frac{\partial u}{\partial t} + \rho(u, \nabla)u = \nabla \left[-PI + \mu \left((\nabla u + (\nabla u)^T) \right) \right] + \rho g + F, \\ \rho \nabla. (u) = 0. \end{cases}$$
(6)

In the equations (6), P is the pressure, u is the fluid velocity, **I** is the three-dimensional unity tensor, μ is the viscosity of the melt. ρg is the gravity force and **F** is the sum of all other body forces. In this work Marangoni force is considered. Values of the temperature dependent density for 316L SS are known from reference[1] as plotted in Figure 3. Using these values of material density, the gravity force F_a is already included in expression (6). Liquidsolid separation in the geometry is reached using a smooth shift of the viscosity from a value of liquid viscosity, in the liquid range, to an infinitely high value in the solid temperature range. SLM being a symmetric phenomenon; plane of symmetry bisecting the laser beam along scanning direction was considered in our single scan model.

Numerical methods

To solve the mathematically defined problem, FE method is used by means of COMSOL Multiphysics Software. A two-ways coupling between Heat Transfer and Fluid Flow is established. The geometry comprises a bulk layer and powder layer with two sublayers of thickness \emptyset and $(1-\emptyset)$. This allows considering change into properties of material after melting of powder and consolidation into a bulk material. The upper part is of relatively higher importance where many phenomena are involved at relatively higher temperature. The meshing of this part is done with extra fine mesh with maximum element size of 12 microns. Figure 2 gives details regarding geometry and meshing.

Results and discussion

Figure 4 presents the velocity field in the molten pool as compared to temperature profile. A scale factor of 1.5×10^{-5} is used. On the top surface, results reveal a movement of the melt generated from the region of highest temperature gradient towards the boundary of the molten pool.



Figure 2. Single scan model geometry and meshing.



Figure 3. Thermal properties of 316 SS.

This movement is accompanied with in heat conduction by convection which expends the size of the molten pool. It can be seen from Figure 5 that a velocity magnitude as high as 2 m/s can be reached.



Figure 4. Velocity field in the molten pool with temperature profile (in K).



Figure 5. Velocity magnitude in the molten pool (in m/s). The red region shows the region of highest velocity.

Molten pool expansion due to heat convection is confirmed in Figure 6. Molten pool sizes are plotted comparing the case where the flow in the molten pool is considered (Figure 6 (B)), and the case where the flow is negated (Figure 6 (A)). The two images are captured at the same magnification and were obtained from the same model geometry and same process parameters. The comparison shows a difference of about 9 microns in the size of the whole molten pool measured on the top surface.



Figure 6. Comparison of the molten pool size in case where the flow is considered and in case it is neglected.

It is worth to note that the size of the molten pool obtained in this simulation might be a little bit

underestimated due to a simple model of laser power deposition used. The volumetric energy deposition model used is commonly used in many simulation works. It is even better than the very simple surface energy deposition model also frequently used. Nevertheless, one should bear in mind that these models do not consider radiation diffraction and multiple reflection on powder particle surfaces and substrate which enlarge the volume of absorption and reduces local power absorption intensity. This note also reflects the maximum temperature on top surface that might be overestimated near the laser position.

Conclusion

Modelling Marangoni effects and flow in the molten pool during Selective Laser Melting is demonstrated on 316 SS material using COMSOL Multiphysics. Due to gradient in surface tension, a shear thermal capillary force acts on the molten fluid and generates movement from the region of highest temperature gradient towards the solidification front. The velocity magnitude is of the order of 2 m/s and causes enlargement of the molten pool as compared to the assumption of a molten pool with no melt flow.

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