Level-set modelling of Laser Beam Melting process applied onto ceramic materials – Comparison with experimental results

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Abstract. Laser Beam Melting (LBM) processes benefit from significant progress in recent years. Currently, manufacturing of ceramic parts for applications at high temperature in aeronautical industries can be planned. However, understanding of defect formation is required in order to optimize manufacturing strategy. In this work, level-set modelling is proposed to simulate tracks development during LBM processes. Thermo-mechanical solution is performed in both powder and dense domains. Fluid flow is computed considering the surface tension and Marangoni forces. In addition mechanical resolution is achieved to investigate stress evolution in the rear part of the track. Applications are developed on alumina material. The influence of laser power, scanning velocity and physical properties are investigated and discussed. Validations of the heat source model are proposed by comparisons of melt pool dimensions and shapes with experimental measurements. A coherent evolution of the track morphology is shown when varying process parameters or material properties.

1. Introduction

In the last decade, Additive Manufacturing (AM) processes have emerged in industries. These processes reduce the time gap between design and manufacturing to deliver parts for direct end-use applications. In addition, they give the possibility to produce complex shapes as limited constraints are imposed on the parts geometry. Different AM processes have been developed by industries with various manufacturing strategies and applications covering polymer, metallic or ceramic materials [1]. Among these processes, LBM appears as attractive for high value-added products as encountered in aerospace, energy or medical industries. In such applications, high level of mechanical properties is required and conventional forming technologies are inefficient to develop expected pieces.

In order to develop part layer by layer, powder is melted in LBM. This is achieved by a laser focused on a narrow domain and moving at large velocity. A track then develops during cooling and solidification stages. Fully dense parts can thus be achieved and near net shape is possible. However, defects like cracks, delamination, porosities or poor surface quality are still encountered and induced by the use of non-optimized process parameters. These defects have detrimental consequences on final properties for direct end-use applications [2] and limit the dissemination of LBM processes. The
required tracks should be regular and free from porosities. Efforts are consequently made to master LBM and achieve expected final properties. Clear improvements in the knowledge and influence of physical mechanisms occurring at the track scale are expected in future years. For that purpose, the development of modelling tools is an answer to the need to provide a better understanding and control of the phenomena impacting track shape and mechanical properties. In addition, such tools would permit to propose optimized process parameters and scanning strategy.

However, less development is made on the application of LBM to ceramics compare to metals. Indeed, ceramics like alumina or zirconia have outstanding mechanical strength and excellent thermal and wear resistance [3]. Nevertheless, some difficulties are known in the application of LBM technologies to ceramic materials explaining this situation. Ceramics have a low energy absorption to Nd:YAG laser used in LBM causing energy loss and reducing production rate. Moniz [4] proposed to overcome low absorption of powders by adding a specific amount of IR-absorbers as carbon or silicon carbides particles. In addition, ceramics have high melting point, high-temperature strength and low thermal conductivity [5]. Cracks formation in solidified tracks are also regularly reported due to the low fracture toughness of ceramics [6,7]. Solutions are proposed in order to limit cracks developments mainly based on powder preheating before melting as developed by Hagedorn [3] on alumina-zirconia (Al₂O₃-ZrO₂) or Liu [5] on zirconia-ytria (ZrO₂-Y₂O₃) ceramics using an auxiliary laser.

In order to provide tools to master and control LBM at narrow scale, a level-set (LS) modelling has been developed and applied on pure alumina powders to follow tracks development [8,9]. Thermomechanical evolution of material is investigated in both liquid and dense domains. Fluid flow evolutions in the melt pool are considered induced by the effects of surface tension and Marangoni forces. The same resolution gives access to the velocity field at the liquid/gas interface and track shape evolution. In addition the mechanical resolution is achieved considering a temperature dependent constitutive law in the solidified domain. This model provides the tools to investigate the influence of process parameters and physical properties of materials on track evolution and defects development.

2. Model

2.1. Level Set Method

The finite-element (FE) model presented in this paper has been extensively described by Chen et al. [8,9,10]. The approach is briefly underlined hereafter in order to describe the points of interest and focus on the originally of the model. The system is made of two domains (material and gas) (Fig. 1a) where powder ceramic is assimilated to a continuum. Material domain is made of pure alumina and corresponds to the powder bed in its initial state before melting. Previous consolidated layers are considered as the substrate domain on which powder layer is deposited. The powder is melted by laser during scanning step and rapidly cooled down by thermal diffusion to form a compact solid domain. During this one-way transformation, densification is modelled through the local apparent density variation from powder to liquid state. The surface evolution then depends from forces acting in the liquid bath. Its evolution is tracked with a LS method depending from the signed distance function, \( \psi \), attached to the material / gas interface. This function is considered as positive (resp. negative) in the gas (resp. material) domain (Fig. 1 a). The Heaviside function, \( H \), is then deduced from the distance function in the whole system and evolves continuously in the transition domain \([-\varepsilon, +\varepsilon] \):

\[
H(\psi) = \begin{cases} 
1 & \text{if } \psi < -\varepsilon \\
\frac{1}{2} \left(1 + \frac{\psi}{\varepsilon} + \frac{1}{\pi} \sin \left(\frac{\pi \psi}{\varepsilon}\right)\right) & \text{if } |\psi| \leq \varepsilon \\
0 & \text{if } \psi > +\varepsilon 
\end{cases}
\]

(1)

The local properties \( \chi^{\varphi,i} \) are computed in each domain \( D_i(i \in \{1,2\}) \) from the intrinsic properties of phase \( \varphi \) (liquid, domain, powder or gas) and of their volume fraction, \( g_{D_i}^{\varphi} \). The system properties \{\chi\}
are then deduced in any position by using the Heaviside function value, \( H \), and the properties associated to each domain. These relations aims at defining the thermo-physical properties and the set of equations averaged over the system corresponding to energy, momentum and mass conservation.

\[
\frac{\partial (\rho h)}{\partial t} + \nabla \cdot (\rho u) - \nabla \cdot (\lambda \nabla T) = \{q_L\} - \{q_r\}
\]  

(2)

The Nd:YAG Gaussian laser source used in LBM provides low interaction with ceramics and pure alumina is considered as transparent with deep propagation contrary to metals. The ceramic powder thickness and several layers are consequently heated. This phenomenon should be limited to prevent large melting/solidification history. Consequently carbon particles (dopants) are added in the powder bed [4] to increase interaction. A continuous modelling is proposed where the local effective laser absorption, \( \alpha \), is considered and the laser heat source, \( \{q_L\} \), is computed from a Beer-Lambert law [11]. For a given depth \( z \), this source is derived from the spatial integration of the local absorption coefficient considering material properties variations. A regular grid covering the impacted domain is used to develop computation (Fig. 1 b) before interpolation onto the initial FE mesh. The radiation loss, \( \{q_r\} \), is estimated assuming a pure radiative heat exchange from the surface.

\[
\frac{\partial \sigma}{\partial t} + (u \cdot \nabla)u - \nabla \cdot \left( \rho \frac{\partial \sigma}{\partial t} \right) = f_s + f_m + \left( \rho \frac{\partial g}{\partial t} \right)
\]  

(3)

\( \sigma \) is the stress tensor and \( g \) is the gravity vector. \( f_s \) and \( f_m \) are the forces associated to surface tension and Marangoni forces applied onto the liquid/gas and liquid/powder interfaces. These forces are respectively developed in the normal and tangential direction of the interface and expressed in (Eq. 4).

\[
f_s = \delta_{ST} \gamma \kappa \mathbf{n}, f_m = \delta_{ST} \frac{\partial \gamma}{\partial T} \nabla_s T
\]  

(4)

\( \delta_{ST} \) is the Dirac function computed onto the interfaces where forces act. \( \gamma \) is the temperature-dependent surface tension coefficient and \( \kappa \) is the curvature radius. \( \mathbf{n} \) is the normal vector to interface.
and \( \nabla \cdot \mathbf{T} \) is the surface temperature gradient. In addition, shrinkage is considered as apparent ceramic density sharply evolves during melting and consolidation of powder. Thus a compressible Newtonian constitutive law is used in the whole system including material and gas domains:

\[
\mathbf{a} = \mathbf{s} - p \mathbf{I} \quad \mathbf{s} = 2\mu \left( \mathbf{\dot{e}} - \frac{1}{3} \text{tr} \left( \mathbf{\dot{e}} \right) \mathbf{I} \right) \quad \text{tr} \left( \mathbf{\dot{e}} \right) = \nabla \cdot \{ \mathbf{u} \}
\]

where \( \mathbf{a} \) is the deviatoric stress tensor, \( p \) is the pressure and \( \mu \) is the dynamic viscosity. The velocity field divergence is estimated from the temporal derivative of the effective density in the expression of mass conservation equation. After resolution, the velocity field is used in the transportation equation to update the position of the distance function and LS interface associated to track shape.

### 2.4. Solid mechanics

In LBM process, the stresses at the track scale are generated by the large temperature gradients and associated density variation during heating and cooling stages. The modeling of solid mechanics consists in the resolution of equilibrium equations associated to momentum conservation as:

\[
\nabla \cdot \mathbf{a} + (\rho) \mathbf{g} = 0
\]

with given boundary conditions corresponding to imposed velocity or normal forces. The modeling of solid mechanics requires consequently a suitable constitutive law which can be used in the full temperature range in order to cover the whole temperature evolution of ceramics. As viscous phenomena become important at large temperature, a general model is required. Three regimes are consequently distinguished on ceramic materials: an elasto-viscoplastic (EVP) behavior at temperature lower than a critical temperature \( T_c \) close to the solidus temperature, \( T_s \), where viscous effects are negligible; a viscoplastic (VP) behavior in the mushy zone between liquidus (\( T_L \)) and solidus (\( T_s \)) temperature and a Newtonian behavior for temperature higher than the liquidus (\( T_L \)).

### 3. Applications and discussion

First applications are proposed in order to follow track development of a 50 µm powder layer deposited on a 1 mm-thick and 3 mm-long substrate. Materials properties of ceramic materials are detailed by Chen et al. [8,9,10]. The first investigation is proposed for a laser power, \( P_L \), of 84 W and a scanning velocity of 200 mm·s\(^{-1}\). Laser interaction radius \( r_{\text{int}} \) is fixed to 50 µm and same absorption coefficient for solid and liquid phase (\( \alpha_s = \alpha_l = 5 \text{ mm·} \text{s}^{-1} \)) are considered. Fig. 2 a) illustrates the evolution of liquid velocity field and melt pool size for various Marangoni coefficients, \( \partial \gamma / \partial T \). Centrifugal convection is observed in first (#1) and second (#2) simulations induced by the negative coefficient corresponding to forces acting in the opposite direction of temperature gradient (Eq. 4). The melt pool is elongated with length close to 400 µm. In the opposite case, centripetal velocities are obtained with a shorter melt pool. In both case, the melt pool is stable and feed by droplets formed in the irradiated domain. In addition, it is observed that Marangoni effect is restricted to the upper part of the liquid bath with few convection in the bottom part due to the high viscosity of liquid ceramic.

The mechanical behaviour has been computed with various strategies in order to investigate additional heating effect on stress distribution (Fig. 2 b). A principal laser is used with \( P_L^{(1)} = 84 \text{ W} \) and \( r_{\text{int}}^{(1)} = 50 \text{ µm} \). Scanning velocity is fixed to 300 mm·s\(^{-1}\) and stress distribution are shown in first case (Single laser). When the material is heated, the density decreases inducing thermal expansion and local compressive stress. Local tensile stresses are observed in upper part which may lead to cracks formation. An additional coaxial laser is used later with lower density energy ( \( P_L^{(2)} = 60 \text{ W} \), \( r_{\text{int}}^{(2)} = 200 \text{ µm} \)) to enlarge the heating zone and control cooling regime. Due to temperature effect, the thermal gradient is reduced and lower tensile stresses are observed. This may limit defect development and provide tracks of better quality. The last case corresponds to the shift of the same auxiliary laser toward the tail at a distance of 250 µm. This configuration affects the tail of the melt pool rather than the front. Consequently, the melt pool is enlarged with a similar depth. As the additional heating is
imposed directly on the melt pool tail, the thermal gradient and cooling rate are reduced. This successfully decreases the stress near the track surface and in the cooling domain. These simulations provide valuable information in the heating strategy to limit defect development in LBM processes.

Figure 2: a) Melt pool (red contour) and liquid velocity field when the laser arrives to position \( X = 1.416 \text{ mm} \) (top view) for various Marangoni coefficient reported in literature equal to (#1) \(- 8.2 \times 10^{-5}\) [12] and (#2) \(- 48 \times 10^{-5} \text{ N m}^{-1} \text{ K}^{-1}\) [13]. An added case (#3) is proposed with \(+ 48 \times 10^{-5} \text{ N m}^{-1} \text{ K}^{-1}\). Irradiated domain is highlighted by the black circle with radius \( r ( r = 1.5 \times r_{\text{int}} = 75 \mu\text{m} )\). b) Stress distribution \( \sigma_{xx} \) (building direction) at \( t = 8 \text{ ms} \) for tree heating strategy: single laser, coaxial laser and shifted laser. White lines correspond to iso-temperature lines in ceramic material.

In addition, comparisons of simulated melt pool shape with observations have been developed based on experimental results produced by LBM on \( \text{Al}_2\text{O}_3 \) ceramic [4,14]. Dedicated experiments were carried out under different laser powers and scanning speeds. Melt pool shape were measured on cross sections for a selected set of process parameters (Fig. 3). A careful calibration procedure has been afterward developed in order to estimate laser interaction radius and absorption coefficients from observations also including an analytical model. Comparisons show good agreements with melt pool depths, \( H_{ZR} \), similar to observations (Fig. 3 a) despite the simplified approach proposed. Numerical shapes are also similar to experiments in particular for medium linear energy (Fig. 3 b).

Figure 3: a) Evolution of melt pool depth, \( H_{ZR} \), as a function of the laser velocity for various power. Comparisons are developed between experiments and numerical simulations for calibrated values \( (r_{\text{int}} = 64.6 \mu\text{m}, \alpha_s = 8.98 \text{ mm}^{-1}, \alpha_t = 3.88 \text{ mm}^{-1} )\) b) Transverse cross section of tracks showing melt pool shape (blue line) and process parameters influence [10] with simulation results (red line).
4. Conclusion

A levet-set modelling of LBM process has been developed to investigate track development. A volume heat source model is applied considering local absorption coefficient of ceramic powder and dense phases. The fluid flow computation considers the surface tension, Marangoni and gravity force effect to estimate velocity field in melt pool. Marangoni effect is highlighted on the flow evolution at the surface of the liquid bath. The mechanical resolution provides also valuable estimation of stress field in the track. The interest of an auxiliary laser to decrease stresses and limit cracks formation is demonstrated. This point may provide optimized scanning strategy for future applications. An experimental comparison is proposed for a single track development and a set of selected process parameters. A calibration procedure is developed in order to estimate unknown parameters associated to laser interaction radius and absorption coefficients. The thermo-mechanical model provides track morphology similar to experimental observations. Melt pool depth show also good agreement with simulations although some differences are visible for low velocity or high power. Future development should consider several superimposed tracks or complex scanning strategy, also including more physical phenomena. Coupling with current developments at macro-scale will also be considered.

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