Modeling of microstructure evolution in direct metal laser sintering: A phase field approach

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Abstract. Direct Metal Laser Sintering (DMLS) is a new technology in the field of additive manufacturing, which builds metal parts in a layer by layer fashion directly from the powder bed. The process occurs within a very short time period with rapid solidification rate. Slight variations in the process parameters may cause enormous change in the final build parts. The physical and mechanical properties of the final build parts are dependent on the solidification rate which directly affects the microstructure of the material. Thus, the evolving of microstructure plays a vital role in the process parameters optimization. Nowadays, the increase in computational power allows for direct simulations of microstructures during materials processing for specific manufacturing conditions. In this study, modeling of microstructure evolution of Al-Si-10Mg powder in DMLS process was carried out by using a phase field approach. A MATLAB code was developed to solve the set of phase field equations, where simulation parameters include temperature gradient, laser scan speed and laser power. The effects of temperature gradient on microstructure evolution were studied and found that with increase in temperature gradient, the dendritic tip grows at a faster rate.

1. Introduction
Direct Metal Laser Sintering (DMLS) process is a type of powder-based additive manufacturing method capable of producing complex structures out of metallic powder in a layer by layer fashion. The process creates three-dimensional solid objects by bonding powdered materials using laser energy [1]. The key advantages of such a layer based fabrication technology over the conventional manufacturing are high degree of design freedom without the need for part-specific tooling, easy processing of powder material, environment friendliness due to minimization of waste and emission, less expense due to absence of support structures [2, 3]. Figure 1 shows the schematic diagram of the DMLS.

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Microstructure is the central core of a material which determines the physical and mechanical properties of materials. For improving the properties of material, it is necessary to control the microstructure of the material as well as the process parameters. But in reality it is very difficult to control the microstructure of the material during experiment. Microstructure evolution takes place to reduce the total free energy that may include the bulk chemical free energy, interfacial energy, elastic strain energy, magnetic energy, electrostatic energy etc. [4]. Due to complex and nonlinear nature of microstructure evolution, numerical approaches have been employed. There are different approaches developed for microstructure modeling. During the past few years, the phase-field approach has emerged as one of the most powerful methods for modeling many types of microstructure evolution in different processes like solidification, solid-state phase transformation, grain growth and coarsening and martensitic transformation etc. [5]. The phase-field method describes the microstructure of a material by using a set of conserved and non-conserved field variables, that are continuous across the interfacial region. An important advantage of this phase-field method is that it considers diffuse interface description, there is no need to track the interfaces during microstructure evolution [6].

Over the past decades few attempts have been made to simulate the microstructure evolution in additive manufacturing processes. Fallah et al. [7] developed a quantitative phase field model for the laser deposition of Ti–Nb alloy. Their model was used to simulate the dendrite growth pattern under thermal conditions i.e., temperature gradient and solidification velocity which obtained from the previously developed thermal model. Rishi et. al. [8] developed a model for the microstructure evolution in selective laser sintering in which a discrete element approach was used, where the particle-to-particle and particle-to-wall mechanical and thermal interactions has been considered. Sahoo et al. [9, 10] developed a quantitative phase field model for the microstructure evolution of Ti-6Al-4V in electron beam additive manufacturing process. The authors used temperature gradient and the solidification velocity as the simulation parameters, which were previously extracted from a thermal model. From the simulation results, the columnar dendritic arm spacing values were estimated and compared with the experimental and analytical results. Montiel et al. [11] studied the microstructure analysis of AZ31 magnesium alloy...
welds by using phase field method. From the simulation they found the condition for columnar to equiaxed transition of dendrites and studied the effect of process parameters on the size and shape of dendrites.

Till date there was no such comprehensive study carried out for the microstructure evolution of laser sintering process. The objective of this study is to apply the phase field method for the microstructure evolution in Direct Metal Laser Sintering process.

2. Phase field formulation
Phase field method is employed to numerically simulate the evolution microstructure of Al-Si-10Mg in DMLS process. The governing equations, when coupled with the temperature and diffusion equations shows the behavior of the interface which is smooth but experiences brisk changes in the phase field. The following assumptions are considered for the phase field model:

i. The constant temperature term is replaced with temperature which changes with time and position, i.e. $T \rightarrow T(x, t)$, where $x$ is position vector and $t$ is time, so as to make the system non-isothermal.

ii. Latent heat of fusion has been neglected and temperature field has been introduced in the form of temperature gradient.

iii. Thermo-physical properties of the system are taken as constants.

iv. Solid/liquid interface is taken to be in local equilibrium.

By using the conserved and non-conserved phase field variables, the governing equations are given by

$$\tau A^2(\varphi) \frac{\partial \varphi}{\partial t} = W_\varphi \nabla \cdot (A^2(\varphi) \nabla \varphi) - W_\varphi \partial_x [A(\varphi) A'(\varphi) \partial_y \varphi] + W_\varphi \partial_y [A(\varphi) A'(\varphi) \partial_x \varphi] - \frac{d g(\varphi)}{d \varphi}$$

$$- \frac{L(T_c - T_m)}{H T_m} \frac{d p(\varphi)}{d \varphi} + \eta'(x, T_c)$$ \hspace{1cm} (1)

$$\frac{\partial T}{\partial t} = \nabla \cdot (\alpha(\varphi) \nabla T) + L h'(\varphi) \frac{d \varphi}{d t} - \frac{\lambda H}{\lambda T_m} \frac{d P(\varphi)}{d \varphi}$$ \hspace{1cm} (2)

where,

$A'(\varphi)$ = derivative of $A(\varphi)$ with respect to the order parameter

$\eta'(x, T_c)$ = stochastic noise function emulating thermal fluctuations

By rescaling space and time as $(\tilde{x} \rightarrow x/W_\varphi)$ and $(\tilde{t} \rightarrow t/\tau)$, we get

$$\varphi^{n+1} = \varphi^n + \frac{\Delta \tilde{t}}{A^2(\theta)} \left\{ \nabla \cdot \left( A^2(\theta) \nabla \varphi - \partial_x [A(\theta) A'(\theta) \partial_y \varphi] + \partial_y [A(\theta) A'(\theta) \partial_x \varphi] \right) - \frac{d g(\varphi)}{d \varphi} - \tilde{\lambda} H \frac{d P(\varphi)}{d \varphi} + \eta'(x, T_c) \right\}$$

$$H^{n+1} = H^n + \frac{\Delta \tilde{t}}{\nabla^2 A^2(\theta)} \Delta^2 H^n + \Delta \tilde{t} h'(\varphi^n) \frac{\varphi^{n+1} - \varphi^n}{\Delta \tilde{t}}$$ \hspace{1cm} (3)

Where $\tilde{D} = a_2 \tilde{\lambda}$, $a_2$ is a constant, $\tilde{\lambda}$ is a rescaled $\lambda$

In the current phase field model, the anisotropy effects are included as given in the following equations,
\[ A(\theta) = 1 - 3\varepsilon_4 + 4\varepsilon_4 \frac{\left( \frac{\partial \varphi}{\partial x} \right)^4 + \left( \frac{\partial \varphi}{\partial y} \right)^4}{|\nabla \varphi|^4} \] …………………………………………………………………………………… (5)

As mentioned in the assumptions, the temperature field was introduced in the form of temperature gradient. The temperature of the molten pool was derived from Echebarria et al. [12]

\[ T(x, t) = T_0 + G(x - V_p t) \] …………………………………………………………………………………… (6)

where,

- \( T_0 \) = reference temperature,
- \( V_p \) = pulling speed in the x-direction
- \( G \) = temperature gradient.

3. Numerical procedures for the phase field simulation

For microstructure simulation the temperature gradient was extracted from the thermal model and integrated in the phase field model. Finite difference method with the central difference scheme was used to solve the governing equations with zero flux boundary condition. To solve the phase field equations, a MATLAB code was developed. The phase field model was carried out by considering the top surface of the powder layer in the build geometry which is in X and Y directions. The heat flux affects the top surface of the powder layer and the microstructural changes occur in this surface. The computational domain was taken with 200 \( \mu \)m \( \times \) 200 \( \mu \)m in both X and Y directions. The domain was divided into 1000 \( \times \) 1000 number of grids with grid spacing of \( dx=dy=0.2 \) \( \mu \)m. The simulations were initialized with a circular seed of radius 5 \( \mu \)m at the center of the computational domain.

The iterations were based on the following procedure:

i. Compute the initial parameters and the phase field variable in the defined domain.
ii. Prepare the order parameters field and start the modeling by enabling the adaptive mesh refinement
iii. Build the anisotropy functions of the order parameters, differentiate them anisotropic order and fix the boundary conditions.
iv. Build the temperature field with order parameters and differentiate them.
v. Solve the phase field equations using the central difference scheme of the finite difference method.
vii. Update the fields using new values and then return to steps (iii) and (iv) for next iteration until the field reaches the boundary.

4. Results and Discussion

There are a number of process parameters which determine the microstructure evolution of the build sample in DMLS process. It is very important to control all these parameters namely solidification growth rate, temperature gradient, chemical composition and the undercooling. Among all these parameters, temperature gradient is one of the most important parameter on which the microstructure evolution depends. The thermo-physical properties of Al-Si-10Mg and the process parameters used for simulation are given in Table 1 and Table 2. The temperature gradient is calculated from the thermal simulation profile shown in Figure 2.
Table-1: Thermo-physical properties of AlSi10Mg alloy [13]

| Properties                        | Values          |
|-----------------------------------|-----------------|
| Thermal conductivity (K)          | 113 W/mK        |
| Specific heat capacity (C_p)      | 940 J/kgK       |
| Convective heat transfer coefficient (h) | 80 W/m²K    |
| Density (ρ)                       | 2.67 g/m³       |
| Emissivity (ε)                    | 0.19            |
| Solidus temperature (T_s)         | 830 K           |
| Liquidus temperature (T_l)        | 869 K           |

Table-2: Process parameters of DMLS process

| Parameters            | Values  |
|-----------------------|---------|
| Laser Power           | 130 Watts |
| Scanning speed        | 500 mm/s  |
| Laser spot size       | 0.2 mm   |
| Thickness of layer    | 1mm      |
| Laser absorptivity    | 0.95     |

Figure 2. 2D view of thermal profile of Al-Si-10Mg powder layer in DMLS

The temperature gradient was calculated based on the correlation [8]

\[ G = \frac{T_{max} - T_l}{r} \] (7)

The main factors for the calculation of the temperature gradient are:
- \( T_{max} = \) the maximum temperature in the melt pool
- \( T_l = \) liquidus temperature of the alloy
- \( r = \) distance between the liquidus line and the spot of the maximum temperature

Based on the above calculation, the temperature gradient for a scan speed of 500 mm/s was found to be 528.27 K/mm. Taking the temperature gradient and the scan speed at 500 mm/s, the phase field simulation is carried out. Figure 3 shows the phase profile of Al-Si-10Mg at different time. At time t=0 sec, the computational domain is initialized with a small solid nucleus having a size of 5 µm placed in the center of the domain. The colour bar of the simulation domain represents constant values, so it has no
unit. In the colour bar, ‘0’ represents completely liquid state and 100 represents completely solid state. At time $t = 50$ ms, the small solid nucleus grows and forms the dendritic arms. With increase in solidification time the dendritic arms grow and finally it grows like columnar structure which is clearly seen in the simulation results. The laser sintering process involves partial melting and solidification phenomena. When the laser beam scans the powder bed, a large temperature gradient created on the powder bed due to the high energy laser beam. This temperature gradient helps to melt the powder particles in the powder bed, then solidify and sinter the powder particles within few fraction of seconds. Due to the melting and solidification, a large temperature gradient exists on the powder bed which helps for the growth of the dendritic arm.

![Figure 3](image)

**Figure 3.** Phase profile of Al-Si-10Mg at different solidification time (a) $t = 50$ ms (b) $t = 300$ ms (c) $t = 1500$ ms (d) $t = 13000$ ms

### 4.1 Effect of temperature gradient on microstructure

The phase field simulations of sintered Al-Si-10Mg are carried out using different temperature gradients. All of these temperature gradients are found using the thermal simulations and the melt pools inhibited by their results. As the temperature gradients have been used prominently in the simulations, one important factor plays a vital role in the final microstructure formation of the materials i.e., cooling rate. The cooling rate which can be described as,

$$ T' = GR \tag{8} $$

Where $G$ = temperature gradient ($K/mm^{-1}$)
\[ R = \text{solidification growth rate (mms}^{-1}\text{)} \]

The cooling rate, being directly proportional to the temperature gradient and the solidification growth rate has a great impact on the microstructure. Any change amongst both of the parameters leads to a change in the final dendritic structure. Increase in the cooling rate tends to extract more heat from the liquid which results in the increase in growth of the dendrites as shown in Figure 4.

![Figure 4](image)

**Figure 4.** Phase profiles of Al-Si-10Mg at different temperature gradients (a) 263.33 K/mm (b) 318.18 K/mm (c) 362.66 K/mm

The phase profile shows at low temperature gradient; the growth of the columnar dendrites is slower as compared to high temperature gradient. With increase in temperature gradient the growth becomes faster and more columnar structure is observed. This is due to the increase in cooling rate with increase in temperature gradient as the scan speed remains constant. As the cooling rate increases, the extraction of heat from the liquid increases which results faster growth.

5. Conclusion
Phase field method was successfully applied for the simulation of microstructure of Al-Si-10Mg alloy in DMLS processes. MATLAB code was used to solve the phase field equations, which incorporates the temperature gradient and laser scan speed as the simulation parameters. As the input to the phase field model i.e., the temperature gradient was extracted from the thermal model and incorporated in the phase field model. From the simulation results it was observed that the temperature gradient plays an important
role for the evolution of microstructure. With increase in temperature gradient, the tip of the dendrites grows faster.

References

[1] Simchi A. 2006, Materials Science and Engineering A.428148.
[2] Kruth JP, Wang X, Laoi T, Froyen L. 2003, Assembly Automation.23357.
[3] Qian B, Shen Z. 2013, J. Asian Ceramic Societies. 1(4)315.
[4] Grong Ø, Shercliff HR. 2002, Progress in Materials Science.47 163.
[5] Chen L. 2002, Annual Review of Material Research.32 113.
[6] Steinbach I. 2009, Modeling and Simulation in Materials Science and Engineering.17 1.
[7] Fallah V, Amoorezaei M, Provatas N, Corbin SF, Khajepour A. 2012, ActaMaterialia. 601633.
[8] Ganeriwala R, Zohdi TI. 2014 Procedia CIRP 14 299.
[9] Sahoo S. 2014, Int. J. Nano and Biomaterials. 5(4)228.
[10] Sahoo S, Chou K. 2016, Additive Manufacturing 9 14.
[11] Montiel D, Liu L, Xiao L, Zhou Y, Provatas N. 2012, Acta Mater. 60 5925.
[12] Echabarria B, Folch R, Karma A, Plapp M. 2005, Physical Review E.72 061604.
[13] Hu H, Ding X, Wang L. 2016, Optik 127 8883.