Numerical Analysis of the Temperature Field during Single-pass Two-layers Laser Additive Manufacturing of Fused Silica Glass

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Abstract. Laser-based additive manufacturing (AM) of glass is rare and complex, which involves highly non-linear thermodynamic problems. The temperature gradient is essential in analyzing the residual stress distribution and thermal deformation. At present, there is no accurate formula to describe the temperature field, and it is also difficult to measure the real-time temperature of the molten pool during the AM process. The numerical method in predicting the temperature field of fused silica glass laser becomes attractive. In this work, a finite element (FE) model for laser AM of quartz glass is established, and the temperature field of laser AM of quartz glass based on the principle of coaxial powder feeding is simulated by combining a moving heat source and birth-death element method. The temperature fields under different laser powers and scan speeds are investigated respectively. Results show that the peak temperature increases with the decrease of laser scan speed and the increase of laser power; The temperature of the upper layer is higher than that of the lower layer because of the heat accumulation effect; The increment rate of laser power and scan speed is set in the range of -12.5% to 37.5% to ensure the temperature of AM region is slightly above the melting point of quartz glass. It is found that the influence of power change on the temperature field is more significant than that of scanning speed. Meanwhile, the peak temperature-dependent linearly on those two variables discussed. The results provided here are instructive for subsequent laser AM of glass material including coaxial powder feeding method, powder cladding, etc.

1. Introduction
Laser additive manufacturing (AM) technology is a manufacturing method that integrates rapid prototyping and laser cladding technology. It has gained particular interest owing to its advantages of material saving, high production efficiency, and low cost [1-6]. In recent decades, with the rapid development of laser AM technology, the range of materials that can be processed has developed from metals [7, 8], ceramics [9, 10], and polymers [11, 12] to the current transparent materials such as glass [13-16]. It is worth noting that its process parameters vary with the performance, application, and material of the product. Sometimes, even if the same material has a different physical state, the corresponding process parameters will vary greatly. Therefore, in large-scale applications, it is costly and time-consuming to determine the adjustment range of its parameters only by experiments. In this
case, it is undoubtedly an ideal alternative to use the FE method to simulate the AM process numerically [17, 18].

Numerical analysis have been widely used to investigate heat transfer characteristics and thermal mechanism of the powder bed fusion (PBF) process [19-25]. In 2009, Roberts et al. [26] utilized the technique of element birth and death to simulate the three-dimensional temperature field in multiple layers in a powder bed. This model took into account practical layer-wise building, processing parameters, nonlinearities produced by temperature-dependent material properties, and phase changes, which can well understand the transient temperature field of multi-layer AM and the thermal interactions of successive layers. A spatially thermophysical-based analytical model is developed by Khorasani et al. [27] to estimate melt-pool temperature, based on PBF process parameters and thermophysical properties of the material. These results are compared with experimentally observed melt-pool depth for IN718 specimens and found to have good accuracy. In fact, specific boundary conditions [28, 29] and suitable heat source models [30-32] are indeed conducive to more realistic calculation and analysis of the thermal behavior of the AM process. Heigel et al. [29] found that the gas flowing during directed energy deposition AM of Ti-6Al-4V would disturb simulation, and they proved this point by experiment. Their work proposed that in addition to free convection, a measurement-based convection model was required into the thermo-mechanical model of the Ti-6Al-4V to obtain accurate simulation results. Furthermore, the residual stress, temperature profile, and deformation behaviors across a variety of process parameters and feed material combinations can be easily predicted by the FE method, which can provide insights into the design and process optimization for the AM processes [33-37]. Ganeriwala et al. [38] presented a method for simulating the residual stress build-up in Ti–6Al–4V parts produced via laser powder bed fusion and developed a material model to naturally capture the strain-rate dependence and annealing behavior of Ti–6Al–4V at elevated temperatures. Results from the thermomechanical simulations showed good agreement with synchrotron X-ray diffraction measurements used to determine the residual elastic strains in these parts. Li et al. [39] analyzed the effects of laser power and laser scan speed on the thermal behavior of AlSi10Mg powder in the SLM process using the FE method. It was found that the cooling rate of the molten pool as the scan speed increased from 100mm/s to 400mm/s was larger than that of the laser power increased from 150W to 300W. In their research, SLM of AlSi10Mg powder was also experimentally performed using the same processing parameters with the simulation, and a low laser power combined with high laser scan speed yielded a low temperature and an extremely short molten pool lifetime, resulting in the occurrence of micropores in SLM-produced parts. It can be seen from the above that up to now, the Numerical modeling of laser AM processes is fairly well established.

Although there are some numerical simulations have been carried out to investigate the thermal behavior during laser processing of metal powders, few works have been discussed on the temperature distribution during AM of glass materials [40, 41]. Fused silica owes irreplaceable position in the modern industry due to its high transmissivity, low coefficient of thermal expansion, and high hardness [42]. Glass has a high melting point and low thermal conductivity, which leads to the formation of pores and cracks during the AM process [1], so it is more challenging to process by AM than the above metal materials. Meanwhile, since the transient temperature field distribution generated by AM is vital for the residual stress and thermal distortion, it is related to the final performance of the AM-processed products [5]. There are many limitations to measure the temperature field with experimental methods yet. Numerical simulation technology provides an effective method for predicting the temperature field during AM process, which can not only help the next step stress field simulation but provide theoretical support for the determination of the processing parameters of laser coaxial powder feeding AM. It has both theoretical and practical significance. In this paper, a FE model of the laser coaxial powder feeding AM process of quartz glass is established using the ANSYS APDL platform. The temperature field of quartz glass laser AM under different laser powers and different laser moving speeds is simulated and analyzed by the method of combining the double ellipsoid heat source and the birth/death element. The results of this article provide a theoretical basis and reference for subsequent optimization (the thermal distortion and residual stress analysis) of the
laser AM process of quartz glass. Besides, to more accurately simulate the temperature field of the laser coaxial powder feeding AM process, the proposed model is based on the following assumptions [17, 39]:

1. Quartz glass material is regarded as homogeneous and isotropic;
2. The densities of the solid and liquid fused silica glass are assumed to be constant;
3. The effect of convection of liquid material in the molten pool is neglected;
4. The heat conduction of the base to the workbench and fixtures is ignored.

2. Theoretical method and model to heat transfer analysis in AM process

2.1. The heat conduction equation and laser energy model

Under the irradiation of laser beam, the surface temperature of the material increases continuously to the melting point of the glass, and laser irradiation makes the material melt into liquid. The essence of the interaction process between laser and quartz glass is the process of absorption, conversion, and transmission of laser energy by the material. This is a very complicated transient heat transfer process.

In the laser AM process, the heat conduction equation is defined as [43, 44]:

\[
\rho C(T) \frac{\partial T}{\partial t} - \rho \left( K_x(T) \frac{\partial T}{\partial x} + K_y(T) \frac{\partial T}{\partial y} + K_z(T) \frac{\partial T}{\partial z} \right) = Q(x, y, z, t)
\]

where \( \rho \) is the material density; \( C(T) \) is the temperature-dependent specific heat capacity; \( T \) is the current temperature; \( t \) is the interaction time; \( K_x(T), K_y(T), \) and \( K_z(T) \) are the temperature-dependent thermal conductivity of quartz glass in \( x, y, \) and \( z \) directions, respectively (\( K_x(T) = K_y(T) = K_z(T) = K(T) \) when the medium is isotropic); and \( Q(x, y, z, t) \) is the body heat source.

For quartz glass, the variation of thermal conductivity and specific heat under different temperature conditions can be described by equations (2) and (3) [43]:

\[
K(T) = \begin{cases} 
0.9786+1.12 \times 10^{-3} T & 300 \text{K} \leq T \leq 1100 \text{K} \\
2.0504+1.177 \times 10^{-4} T & 1100 \text{K} < T \leq 2100 \text{K}
\end{cases}
\]

\[
C(T) = \begin{cases} 
35.936 + 3.3688T - 0.0041T^2 + 2.5803 \times 10^{-8}T^3 - 8.0867 \times 10^{-11}T^4 + 9.9048 \times 10^{-14}T^5 & 273 \text{K} \leq T < 1973 \text{K} \\
1273 \times 10^{-11}T^2 + 1273 \times 10^{-14}T^3 & 1973 \text{K} < T < 3180 \text{K} \\
1273 \times 10^{-11}T^2 + 1273 \times 10^{-14}T^3 & 3180 \text{K} \leq T \leq 3185 \text{K} \\
1273 \times 10^{-11}T^2 + 1273 \times 10^{-14}T^3 & T > 3185 \text{K}
\end{cases}
\]

where \( L \) is the latent heat of vaporization and is equal to \( 1.23 \times 10^7 \text{J/Kg} \).

If the powder is to be tightly combined with the substrate, the laser must act on the fused silica powder and the glass substrate at the same time in the laser coaxial powder feeding AM process, which requires the laser to have greater penetration and energy. Here, Goldak’s double-ellipsoidal heat source is used in this paper. The power density distributions of the front and rear half of the moving heat source model are described in equations (4) and (5) [45]:

\[
Q_f(x, y, z, t) = \frac{6 \sqrt{3} f_f \eta P}{\pi \sqrt{\pi} a_f b c} \exp \left[ -3 \left( \frac{x^2 + y^2 + z^2}{a_f b c} \right) \right]
\]

\[
Q_r(x, y, z, t) = \frac{6 \sqrt{3} f_r \eta P}{\pi \sqrt{\pi} a_r b c} \exp \left[ -3 \left( \frac{x^2 + y^2 + z^2}{a_r b c} \right) \right]
\]

where \( f_f \) and \( f_r \) are the fractions of the heat deposited in the front and rear halves of the heat source, and \( f_f + f_r = 2 \); \( \eta \) is the absorption efficiency of the quartz glass and \( P \) is the laser power; \( a_f \) and \( a_r \) are the front and rear lengths of the heat source along the direction \( x \) while \( b \) is the depth along the direction \( y \).
and $c$ is the half-width of the heat source along the direction $z$. The parameters of the moving double-ellipsoidal heat source model are listed in Table 1.

| Parameters | Value |
|------------|-------|
| Temperature /K | 298, 373, 523, 773, 1273, 1773, 1973, 2773, 3273 |
| Specific heat /J·kg⁻¹·K⁻¹ | 740, 800, 987, 1100, 1211, 1480, 1500, 1621, 1700 |
| Thermal conductivity /W·m⁻¹·K⁻¹ | 1.3, 1.4, 1.56, 1.84, 3.6, 4.9, 6.7, 13.5, 21.8 |
| CTE (10⁻⁷·K⁻¹) | 2.76, 5.5, 7.95, 5.75, 5.56, 5.1, 6, 11.45, 13.67 |

2.2. Thermophysical parameters of fused silica

The density of quartz glass is 2200kg/m³, the melting point is 1973K, and the vaporization point is 3180K [43]. The coaxial powder feeding method is used to cladding quartz glass powder. It is assumed that the filler material and the base material have the same physical and chemical properties with satisfying isotropy. $c$ and $k$ value changes with temperature and its thermophysical properties are shown in Table 2.

2.3. FE model establishment

A simulation model consisting of two 1mm layers of quartz glass powder is presented in our work. Numerical simulation is employed using the ANSYS APDL finite element analysis package. The SOLID70 has 8 nodes solid element with a 3-D thermal conduction capability, which applies to a 3D steady-state or transient thermal analysis. While SURF152, a 3-D thermal surface effect element, may be flexibly used for various load and surface effect applications. When heat flux and heat convection boundary conditions are applied to the same surface at the same time in ANSYS APDL, one must be applied to the surface of the solid element and the other to surface effect element. So, the SOLID70 hexahedron element is selected in our paper to analyze the temperature field of the fused silica, and the SURF152 element is used for convection load. The FE model and laser scanning pattern during the AM process are shown in Figure 1. The geometric size of the quartz glass substrate has a length of 50mm, a width of 30mm, and a thickness of 5mm. the dimensions of the cladding layer are 50mm×2mm×1mm. In the process of FE simulation, an adaptive meshing strategy is used for the model. That is, the meshes of the laser action area such as the deposition layer and the heat-affected zone are relatively dense (the mesh size is 0.4mm×0.4mm×0.3mm), whereas the meshes far away from the AM area are sparse, which ensures the calculation accuracy and reduces the calculation time of the model also improves the calculation efficiency. The three-dimensional simulation model has meshed into 33879 nodes and 152739 elements. A 10% convergence test was considered to check the convergence of the meshing. The method of element birth and death is used to simulate the formation process of the material in the process of AM. The deposition and generation of the fused silica powder are analogous with the activation of new elements at the corresponding time points [26, 35]. Before the beginning of the analysis, all elements of the AM layer are deactivated ("dead") [35]. Although the elements are visual, their material properties are scaled to be smaller (close to 0) so that they do not affect the analysis before being activated [29]. Only when the laser irradiates the area, the properties of an element are switched from "death" to "birth" (active). At this time, the material properties of the element are restored to participate in the calculation. this process is repeated until the end of the laser coaxial powder feeding AM.
Figure 1. (a) Finite element model and mesh generation and (b) reverse depositing direction of AM process.

To simulate the laser scanning, the double ellipsoid model is used to describe the laser moving heat source. To ensure that the quartz glass reaches the melting point of the laser irradiation area, the laser power is set to 70W-110W, the moving speed is 0.875mm/s-1.375mm/s, and the spot size is 2mm. The appropriate initial and boundary conditions are necessary for the simulation. So set the initial condition of the substrate and fused silica powder as $T(x, y, z) \mid _{t=0} = T_0$, where $T_0$ is the ambient temperature of 25℃. For the laser irradiation area, the thermal boundary condition is as follows:

$$-k \frac{\partial T}{\partial n} = Q(x, y, z, t) - h_{\text{con}} (T - T_0) - \varepsilon \sigma (T^4 - T_0^4)$$

Moreover, considering the general effect of radiation and convection on the surface of the AM-processed parts, the combined heat transfer coefficient as follows is used to replace the convection coefficient [46]:

$$h = \frac{\varepsilon \sigma (T^4 - T_0^4)}{(T - T_0)} + h_{\text{con}}$$

In equations (6) and (7), $k$ is the thermal conductivity coefficient; $n$ is the normal vector of the outer surface; $h_{\text{con}}$ is the convective coefficient, $h_{\text{con}}$ can be set as 8Wꞏm⁻²ꞏK⁻¹; $T$ is the surface temperature of the irradiation area; $\varepsilon$ is the emissivity coefficient of quartz glass and applied to the value of 0.9; $\sigma$ is the Stefan-Boltzmann constant.

For other surfaces that are not irradiated by the laser, only the convection heat loss between the material surfaces and the surrounding environment is considered:

$$-k \frac{\partial T}{\partial n} = h_{\text{con}} (T - T_0)$$

Finally, based on the above theory and the FE package ANSYS APDL, the temperature field distribution under different laser power and scan speed are obtained.

3. Results and discussion

The temperature field of fused silica during laser AM is simulated by FE analysis software, and the s-shaped route is used to simulate two layers of cladding, i.e., single-pass two-layers laser AM of fused silica glass. Figure 2a and 2b are the temperature fields of the first and the second layer over 106s. It can be seen from Figure 2 that the temperature of the laser irradiation point rises rapidly to the melting
point of fused silica within one second. The peak temperatures of all points are higher than the melting point of quartz glass powder, which proves that the powder from the coaxial powder nozzle can be completely melted to form a cladding layer in AM process.

Figure 2. Temperature field of the sample under different time: (a) first layer at 1s, 25s, and 50s (the laser power is 80 W and the moving speed is 1 mm/s); (b) second layer at 54s, 80s, and the last moment.

To further understand the temperature variation during the AM process, we have extracted the temperature cycle curves of each point on path 1, path 2, and path 3. As shown in Figure 3b, 5 points (C', F', F, F'', G'') are taken as path 1 on the plane of $x = 25$ mm, another 4 points (C', C, C'', H1) are taken along the longitudinal (on the plane of $y = 15$ mm) as path 2, and 10 points (A, B, C, D, E, E', D', C', B', A') at the beginning, middle and end of the first AM layer and the second layer are taken as path 3 (shown in Figure 3a).

The thermal cycle curves in Figure 4a are obtained by randomly taking points on path 1. Points C' and F' of the 2nd layer are single peak. The other nodes (F, F', G'') have two peaks, in which the first peak is the heating and melting process of fused silica, and the second peak can be explained by the heat conduction and remelting process of the first cladding layer when the heat source passes through the second layer during the laser AM process.

It can be seen from Figure 4b that apart from point C', points C, C'', and H1 appear two peaks. The peak temperature of the first peak of point C, C'', H1 is 2207.5K, 1519.7K, and 1015.8K, and the peak temperature of the second peak is 2145.5K, 1197.3K, and 917.9K respectively. It is not difficult to see that the temperature of the laser action point is higher than that of the heat-affected zone. For each point on path 3 (Figure 4c), the temperature of the first peak of points A, B, C, and D of the first cladding layer is 2268.9K, 2204.4K, 2207.5K, and 2236.4K, and the peak temperature of the second peak is 2404.2K, 2093.6K, 2145.5K, 2121.7K, and 2242.5K, and the temperature at the points E', D', C', B' and A' on the second layer is 2537.7K, 2449.1K, 2365.6K, 2424.1K, and 2701.5K respectively. With the increase of time, the temperature of the points (except the first and last two points) on path 3 gradually stabilized within a certain range. And the overall temperature of the second layer is always higher than the temperature of the first layer which is caused by the heat accumulation effect. It should be noted that because the geometrical parameters ($a_f$, $a_r$) of the frontal ellipsoid and the rear ellipsoid are different, the time to stay at the corresponding point is different, and the point A' receives more heat than point A. Point A' naturally conducts more heat to the second peak of point A, so it is reasonable that the temperature of the second peak of point A is higher than the temperature of the first peak. In a word, the temperature change trend of the points on path 2 is similar to that of path 3, but the temperature gradient of path 3 is relatively smaller and more uniform than that of path 2. This is because the distance between the nodes of path 2 is much larger than that of path 3, and the thermal
conducivity of quartz glass is extremely small \(10^{-7}/K\), so the heat transfer distance is limited within a certain time.

Figure 3. Schematic diagram of AM path and picking point.

Figure 4. Thermal cycle curves of on (a): path 1(C', F', F, F'', G''), (b): path 2 (C', C, C'', H1); and (c): path 3(A, B, C, D, E, E', E', D', C', B', A') in case of 80W power.

3.1. Influence of laser power on temperature field in AM
As in Figure 5, a thermal cycle curve of the midpoint C of the first cladding layer and its counterpart C' of the second layer during the AM process. In the process of increasing the laser power from 70W to 80W, 90W, 100W, and 110W, the first peak temperature of point C increases from 2106.3K to 2207.5K, 2355.6K, 2462.8K, and 2562.7K, and its second peak temperature increases from 1967.2K to 2145.5K, 2220.6K, 2330.1K, and 2429.9K. Similarly, the temperature of point C' increased from
2229.4K to 2365.6K, 2487.7K, 2600.8K, and 2701.0K, respectively. Apparently, the temperature of the laser irradiation point is gradually increasing with the increase of power. On the other hand, with the increase of laser power, the heating rate increases, and the cooling rate decreases. This is because the thermal diffusion of quartz glass is slow during the interaction between laser and quartz glass, resulting in a lot of energy accumulated at the laser action point. As we can see, in the stages II and IV of the curve (Figure 5), after the heat source passed, the temperature decreases slowly under the combined action of heat dissipation and heat transfer. At the same time, it can also be seen that the heating rate (in the stages I and III of the curve) is higher than the cooling rate. The temperature rises quickly due to the heating process when the material is not yet cladded, the element is "death" and the thermal properties of the material can be deemed as infinitely small (close to 0), and there is no heat conduction. When the element changes from the "death" state to the "birth" state, the thermal properties of the material are activated, at this time there is heat conduction, and there is mutual heat conduction between all elements, so the cooling rate is relatively gentle.

Figure 5. Thermal cycling curves of point C (a) and point C' (b) under different laser power.

The temperature distribution of the first layer at the same time (path 3) is concluded in Figure 6a, the temperature rises sharply at first, up to 2819.3K (when the laser power is 110W), and it lowers slowly as the heat source getting further away. As predicted, the temperature increases with the laser power increase, and the stable linearity can be overserved. Moreover, within the 106s time range, the temperatures reach 505.1K during the cooling process after the laser radiation is moved, and if the time is long enough, it will drop to room temperature. The temperature distribution on the substrate is also important, which is related to the bonding strength between the powder and the substrate. Therefore, 19 points are selected from point C'' to point H'', and the temperature field distribution is shown in Figure 6b. When the power is 70W and 80W, the temperature of the joint between the AM part and the substrate is 1735.8K and 1883.2K, it does not reach the melting temperature of quartz glass. While the laser power is 90W, it reaches 2002.9K, so the laser power above 90W is one of the necessary conditions to produce a good bonding strength.
Figure 6. (a) The temperature distribution of the 1st layer (path 3) under different laser power and (b) the temperature distribution of 19 points from point C'' to point H'' at t=26s.

Here, taking 80W as the benchmark, the change rate of temperature with laser power and laser speed has been got. Under the same laser power, the temperature change rate between the nodes of each layer keeps constant. In the case of the laser power 90w, the peak temperature change rates are 5.26%, 5.58%, and 5.17% respectively. When the power varies from 70W to 110W, the temperature change rates of the first peak of the first cladding layer are -5.88%, 5.26%, 10.05%, and 14.60%, respectively (see in Figure 7). That is, when the laser power increases, the temperature change rate keeps a good linear relationship.

Figure 7. Temperature change rate with laser power and laser moving speed.

3.2. Influence of laser scanning speed on temperature field in AM

It can be seen from Figure 8 that, unlike the thermal cycle curves under different powers in the previous section, the node where the peak temperature occurs at different speeds is no longer the same one, but changes with the change of speed (given the previous section the reason for the formation of the double peaks in the first layer has been explained, so it is not be repeated here). At this time, the faster the laser moves, the smaller the peak temperature will be. It can be seen from Figure 8a that the peak temperature of the first peak is 2169.5K, 2155.2K, 2118.5K, 2102.4K, and 2089.5K respectively when the velocity changes between 0.875-1.375mm/s, showing a decreasing trend. At the same time, the temperature of the second peak will also decrease with the increase of velocity (1972.7K, 1940.4K, 1911.4K, 1890.7K, and 1811.8K respectively). And we can also see that at the same speed, the temperature rise-and-fall time of the second peak is longer than that of the first peak. This is due to the formation of the second cladding layer and the moving of the heat source at that time, and it is still in a
high-temperature state. It can be regarded as a secondary heat source. The cladding layer below will be heated by this secondary heat source for a while until the temperature between these two layers is in equilibrium. In addition, the thermal conductivity of the quartz glass itself is very small, so the heat transfer rate is much slower than that of the first peak. The peak temperature of the counterpart in the second layer also decreases slightly with the increase of speed. Besides, comparing Figure 7 shows that within the same range of rate of change, the influence of speed changes on the temperature field is much smaller than the influence of power changes on the temperature field.

Figure 8. Thermal cycling curves of the 1st layer (a) and 2nd layer (b) under different laser scan speed.

4. Conclusion

In this paper, the temperature field of the AM of quartz glass is simulated and analyzed. The birth-and-death element is used to simulate the material generation process in AM. By individually changing the two parameters of laser power and laser moving speed, their effects on the temperature field of the AM process are obtained. The following conclusions were drawn:

1. In the process of AM, the temperature of the upper layer is higher than the temperature of the lower layer due to the effect of heat accumulation. At the same time, the top layer only has the stage of heating and melting, but the lower layer will experience the stage of heating and melting and remelting produced by the upper layer's heat conduction;

2. When the laser power is 70-110w and the moving speed is 0.875-1.375mm/s: as the power increases, the peak temperature of the laser radiation point gradually increases; as the scanning speed increases, the peak temperature of the laser radiation point slightly decreases;

3. When the change rate of laser power and scanning speed is in the range of -12.5% to 37.5%, there is a linear relationship between them and the temperature change rate;

4. Under the above available parameters, the peak temperature of the laser irradiation point can rapidly rise to the melting point of quartz glass, which can make the AM process stable.

The simulation results in this paper are helpful for us to better understand the heat transfer process of quartz glass AM. In addition to laser power and laser moving speed, other factors (such as spot size, defocusing amount, preheating temperature, etc.) are also important factors affecting the AM process. Therefore, the analysis of their influence on the temperature field of AM process and the stress field analysis of quartz glass AM will be a part of our future work.

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