Numerical Simulation of temperature field distribution for laser sintering graphene reinforced nickel matrix nanocomposites

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Abstract: Transient temperature field distribution is important for quality control of laser sintering graphene (Gr) reinforced nickel matrix (Ni-Gr) nanocomposites and the optimization of sintering parameters. To date, it is difficult to measure the temperature field directly. Thus, numerical simulation was utilized to study the distribution and evolution of temperature field. Finite element models were employed to simulate the sintering process of Ni-Gr coatings on AISI 4140 steel. The temperature distribution, the depth of the melting pool, the width of metallurgical bonding and the parameter optimizing method for laser sintering were investigated. In order to verify simulation results, single-track experiments were performed with the same laser sintering parameters as simulation. Simulated results reveal that convection and radiation heat transfer, and the latent heat of phase transition play a major role in the sintering process. Simulation output is consistent with experiments under the same processing parameters. Based on simulation results, substrate melting depth, metallurgical bonding width and thermal accumulation effects can be predicted. Thus, according to these guidelines, the optimal laser sintering parameters can be decided.

Keywords: Numerical simulation, Laser sintering, Temperature field, Nanocomposite

1. Introduction

Laser sintering has been widely used in many fields, such as rapid prototyping and rapid manufacturing [1], laser synthesis of functional coatings based on composite metallic and metal/ceramic powder mixtures [2-6], and renovation and repairing of critical parts [7]. Laser sintering is rapid heating and cooling process, thereby difficult to measure its temperature field distribution directly at present. However, the temperature field plays a critical role in solidification process, dominating the microstructure and mechanical properties of laser sintered structures. Therefore, numerical simulation has been widely employed to study the temperature field distribution [8, 9], recently. Herein, based on the commercial FEA software, the finite element models of laser sintering Ni-Gr nanocomposites were explored. The effects of laser sintering parameters (laser power P, scanning speed V, spot diameter D) on temperature field distribution were studied. The simulation results were verified by laser sintering experiments.

2 Establishing the finite element model of laser sintering process and experiments

2.1 Mathematical model

AISI 4140 steel plate was used as substrate [10-12]. The coating layer contained 90 wt. % Ni and 10 wt. % graphene. The substrate plate sizes in 14 mm×10 mm×2.35 mm; the thickness of coating layer was 0.1 mm. Fig. 1 is the schematic of laser sintering simulation model.

Fig. 1 Schematic of laser sintering process

Thermophysical properties as a function of temperature, phase transition latent heat, convection and radiation were counted in the FEM model [13]. To simplify the simulation process, it was assumed that: a) the coating materials and substrate are continuous and isotropic, b) neglecting the flowing of melting pool and evaporation of sintered materials, c) laser absorption does not change with temperature.

2.2 Laser heat source

The laser mode is TEM₀₀. The energy density exhibits Gaussian special distribution. The intensity distribution in the Gaussian beam can be expressed as [14]:

$$I(r, 0) = I_0 \exp\left(-2 \frac{r^2}{\omega^2}\right) \quad (1)$$

where r is the radius of the beam, I_0 is the intensity of the beam at $r = 0$ and ω is the radius of the beam at which $I = I_0 e^{-2}$.

During laser sintering process, laser spot was moving continually. The movement based on the discretization method of finite element, using small distance jumping heat source to replace the continuous laser scanning, which means the laser spot moved a unit distance each time. When the laser spot moved to next position, the laser load on the previous position was removed.

2.3 Thermophysical parameters

Table1-3 shows thermophysical parameters of Nickel, graphene and AISI 4140 steel. Linear interpolation method was used to determine the unknown values. The thermophysical parameters of graphene nickel coating layer was calculated from the data listed on table 1 and table 2. For the thermal conductivity of coating composite can be expressed as following[15].

$$K_c = K_g \left\{ K_m \left(3 - 2 f_g \right) + 2 f_g \right\} / \left\{ f_g K_m \left(K_g - f_g \right) \right\} \quad (2)$$

where f_g is the volume fraction of graphene and K stands for thermal conductivity, with subscript c for the composite (Ni-Gr), g for graphene, and m for matrix of Ni. The parameter a is a coefficient relate to matrix material and graphene platelets size. The thermophysical parameters of graphene were assumed to be constant with respect to temperature. Law of mixtures was applied for density and specific heat of the coating layer.

Table 1 Thermophysical parameters of coating layer(Ni)[16]

Melting point/°C: 1453	Density/(kg·m ⁻³): 8.902
Temperature/K	500 550 600 1250 1300 1350
Thermoconductivity/(W·m ⁻¹ ·K ⁻¹)	72.2 68.9 65.6 76.2 78.3 80.4
Specific heat capacity /(J·kg ⁻¹ ·K ⁻¹)	529 534 540 620 616 629

Table 2 Thermophysical parameters of coating layer(Graphene) [17]

Melting point/K: 4900	Density/(kg·cm ⁻³): 1.06
Temperature/°C	20
Thermoconductivity/(W·m ⁻¹ ·K ⁻¹)	4840[18]
Specific heat capacity /(J·kg ⁻¹ ·K ⁻¹)	700 [19]

Table 3 Thermophysical parameters of substrate (AISI 4140)[20]

Melting point/°C: 1416	Density/(kg·m ⁻³): 7.85
Temperature (°C)	25 100 200 300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 1600 1700
Specific heat (J/kg°C)	473 485 496 512 529 541 556 579 594 619 635 664 682 703 726 747 764 781
Thermal conductivity (W/m°C)	42.7 43.2 43.61 45.31 47.01 48.71 50.41 52.11 53.81 55.51 57.21 58.91 60.61 62.31 64.01 31 33.08 35.64

2.4 Geometric model and mesh

In FEA, normally finer mesh results in more precise simulation results, however finer mesh means more elements in the same model size, which will cost more computer resource and calculation time. Herein, for the whole model, coarse mesh was applied, meanwhile, the laser sintering area was refined by small size elements, so that precise results can be accomplished at a low calculation cost. Smaller mesh size provides similar results for test simulation run, which confirms the choice of current mesh size to be sufficient.

Fig. 2 FEM model of laser sintering Ni-Gr composites

2.5 Governing equation and boundary conditions

Considering the latent heat of phase transformation, the partial differential equation for the heat conduction during the laser sintering process can be expressed in its most general form as [21]:

$$k_e \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + q = \rho c \frac{\partial T}{\partial t} \quad (3)$$

where, k_e , ρ and c are the thermal conductivity, density and thermal capacity, respectively. T is the temperature. q is the latent heat of phase transformation and t is time.

The initial temperature was assumed to be 26.85 °C

$$T(x, y, z, 0) = T_0 \quad (4)$$

Due to high temperature at laser point, heat transfer through radiation cannot be ignored. The effect of convection and radiation heat transfer should be comprehensively considered [22]. At top surface, the following boundary condition is governing:

$$-k_e \left. \frac{\partial T}{\partial z} \right|_{z=0} + h(T_s - T_{ext}) + \sigma \varepsilon (T^4 - T_{ext}^4) = q \quad (5)$$

where, T_s is coating layer surface temperature, T_{ext} is the environment temperature, h is convection coefficient, σ is Stefan - Boltzmann constant, ε is radiation coefficient.

For other surfaces:

$$-k_e \left. \frac{\partial T}{\partial z} \right|_{z=0} + h(T_s - T_{ext}) + \sigma \varepsilon (T^4 - T_{ext}^4) = 0 \quad (6)$$

2.6 Phase transition

The latent heat of fusion and solidification were taken into account in this simulation. During the laser sintering process, latent heat can be calculated by:

$$H = \int \rho C(T) dT \quad (7)$$

where H is latent heat of phase transition, ρ , C and T are density, specific heat capacity and absolute temperature, respectively.

2.7 Experiments

The AISI 4140 low-alloyed structural steel plate was cut into small pieces sizing in 14 mm×10 mm×2.35 mm. Microscale nickel powder, graphene nanoplatelets were used to make solution via magnetic stirring by mixing 1.8g nickel powders, 0.2g graphene nanoplatelets and 46g deionized water. Coating was done with ink dropping of mixture solution on metal plate surface, followed by room temperature drying [3-6]. Laser parameters applied in sintering process were the same as FEA.

3 Results and discussion

3.1 Single-track simulation results

Laser sintering parameters used for simulation were: laser power 100 W, laser spot diameter 0.8 mm, scanning speed 2 mm/s, laser absorptivity of coating layer 0.8, initial temperature 26.85 °C (300K). Fig. 3 represents the basic contours of temperature field during laser sintering at 2s, 3.5s, 5s. Overall shape of temperature field on the surface looks like a comet, instead of a circle, which indicates the beam movement direction. Since laser scanning speed was still relatively low, thereby the high temperature spot in the middle was still kept in nearly circular shape. In the laser sintering area, if the temperature achieve above 1453 °C (melting point of nickel), and the nickel powder would be melted to form melting pool.

Fig. 3 Contours of laser sintering temperature field at different time.

(a) 2 s, (b) 3.5 s, (c) 5 s

In Fig. 4, temperature gradient shows uniform distribution around the beam center. The isothermal line is circular around the center of beam, which should be attributed to the slow movement of laser beam. If the laser beam moves fast enough, it should have an obvious comet shape even in the central region [23]. On the plane of symmetry and cross section, the melting depth can be determined. It can be seen that the melting depth was not deep enough to make fully metallurgical bonding between coating layer and substrate.

Fig. 4 Contours of laser sintering temperature field on different surface at 3.5 s. (a) top surface
(b) cross section at highest temperature point (c) symmetry surface

Fig. 5a is the temperature distribution along the central line of the scanning path on the top surface (Line A) and the projection of Line A on the substrate surface at 3.5s. At this time the laser beam center was at the middle of the scanning line (5mm), and it can be seen that the highest temperature point is located in the center of laser beam. It can be measured from the temperature contours, the width of the area where the temperature was higher than 1453 °C, is 0.57 mm. Fig. 5b shows the temperature distribution curve along the long axis on the surface of coating layer (Line B) and the projection of Line B on the substrate surface. The metallurgical bonding area can be measured from temperature distribution curves. For The area with temperature higher than 1453°C, the measured width is 0.05 mm. Fig. 5c shows the temperature distribution along the depth direction (Line C) under laser beam. It can be seen that the temperature gradient is high, temperature changes from 2237°C to 420°C in 2.45 mm. From the contours on this cross section, it can be characterized that whether the substrate and the coating layer have metallurgical bonded, and the depth of melting pool. It can be found that at 0.11 mm deep, the temperature is about 1453°C. This means coating layer was totally melted in the whole depth. Metallurgical bonding was realized, but the width is small, if full metallurgical bonding was required, the higher laser

power would be needed.

Fig. 5 Temperature distribution on different line at 3.5 s.

(a) Line A, (b) Line B, (c) Line C, (d) schematic of selected lines

Fig.6a is the schematic of line A, line B, line C and selected points on these lines. Fig.6b shows the thermal cycle curves of the five points on the center line of scan path (Line A, distance from front surface for Y1、Y2、Y3、Y4、Y5 are 1、3、5、7、9 mm, respectively). It is expected to achieve the highest temperature when the laser beam passes through each point. Maximum temperature for points increases as stored heat ramps up with time. It is due to thermal accumulation during laser scanning process. Fig.6c shows the thermal cycle curves of five points along central line (X axis, Line B) on the top surface (distance from front surface for X1、X2、X3、X4、X5 are 2、2.4、2.8、3.2、3.6 mm, respectively). Before the laser beam approaching Line B, the temperature of these points increases slowly. Then, when the laser beam reached Line B, the temperature change amplifies. The highest temperature for these points decreases as the distance from the point X1 increases. It is shown that maximum temperature for these points is reached one after another, due to time required for heat to travel. Fig.6d shows the thermal cycle curves of points in Z direction (Lin C, distance from top surface for Z1、Z2、Z3、Z4、Z5 are 0、0.4、0.8、1.2、1.6 mm, respectively). Similar to Fig. 6c, before laser approach, the temperature of these points increases slowly. On the other hand, when the laser beam reached the Line C, temperature

increases abruptly. Maximum temperature of these points decreases as distance from the top surface increases. Based on simulated temperature trends, it can be concluded that temperature is relatively high even after passing the peak temperature. It proves that sample temperature would change dynamically as the sintering process continues.

Fig .6 Thermal cycles of selected points during laser sintering

(a)Schematic of location of selected points (b) Line A (c) Line B (d) Line C

3.1.1 Effect of laser power on the temperature field

Table 4 shows the simulation results under the same parameters as used above with 3 different laser powers at 3.5s. As the laser power increases, the peak temperatures , as well as depth of melting pool goes up. Laser power changing brought significant effect on melting pool depth. Specifically, when the laser power was low, increasing laser power had significant effect on the metallurgical bonding, however, after the laser power reached a critical value, further increasing laser powder would cause vaporization of laser irradiated material , this might degrade whole laser sintering quality.

Table 4 Simulation results under different laser power at 3.5s

Simulation	Sim-P1	Sim-P2	Sim-P3

Laser power/W	60	80	100
Highest temperature of coating layer surface/°C	1377	1852	2237
Highest temperature of joint surface/°C	1050	1280	1460
Depth of melting pool/mm	0	0.08	0.11
Width of metallurgical bonding at joint surface/mm	0	0	0.05

3.1.2 Effect of scanning speed on the temperature field

Table 5 shows the simulation results under the same parameters with 3 different scanning speeds. As the scanning speed increases, the peak temperature, as well as depth of melting pool decreases. Comparing to the effect of laser power change, the effect of scanning speed variation were relatively of less significance.

Table 5 Simulation results under different scanning speed

Simulation	Sim-v1	Sim-v2	Sim-v3
Scan speed/ $\text{mm} \cdot \text{min}^{-1}$	1	2	4
Highest temperature of coating layer surface/°C	2420	2237	2024
Highest temperature of joint surface/°C	1485	1460	1420
Depth of melting pool/mm	0.15	0.11	0.09
Width of metallurgical bonding at joint surface/mm	0.35	0.05	0

3.2 Multi-track laser sintering temperature field simulation

Experimentally, almost of real-world laser sintering processes are multi-track sintering. During the multi-track laser sintering process, because of thermal accumulation, the conditions of sintering process are changing constantly. This will make the sintering process more complex, so it is necessary to simulate the process and find out the optimal parameters.

3.2.1 Simulation model

Similar to above, AISI 4140 structure steel plate was used as substrate. 90wt. % Ni and 10wt. % graphene mixed materials were used as coating layer. The substrate plate size is 14 mm $\times$ 10 mm $\times$ 2.35 mm; the thickness of coating layer is 0.1 mm.

Fig. 7 Schematic of multi-track laser sintering process

3.2.2 Geometric model and mesh

Same as single-track simulation model (Fig. 2), multi-track simulation model was created with experimental parameters. For meshing, element size increases from surface of sintering area with finest elements to fine elements for higher 0.2 mm of substrate and coarse elements for the rest of substrate. This method helps to get reasonable results in acceptable amount of simulation time.

3.2.3 Results and discussion

Laser moves back and forth along the X direction, while moving stepwise in Y direction with step size of 0.25mm at the end of each cycle. As shown in Fig. 7, three tracks were selected, point

1($t=3s$), point 2($t=283s$), point 3($t=557s$) are near middle points of the three tracks. The laser sintering parameters used for simulation are: laser power 80 W, laser spot diameters 0.8 mm, scanning speed 2 mm/s, laser absorptivity of coating layer 0.8, initial temperature 300K, and continuously scanning. The total scan time of all tracks is 560s.

Fig. 8 is the thermal contours of laser sintered sample at 3s, 283s, 557s. As laser scanning goes on, the heat affected zone expands. The lowest and highest temperatures of the sample are increased. Minimum temperature increases significantly, which was 44.9°C, 436°C and 402°C at 3s, 283s and 557s respectively; meanwhile, the Maximum temperature increases less. Significant rise in minimum temperature is due to small sample size and slow scanning speed. During the laser sintering process, heat accumulation increases the overall sample temperature.

Fig. 8 Temperature field of multi-track laser sintering at different time

(a) 3s (b) 283 s (c) 557 s

Fig. 9a shows temperature distribution curves along center line of laser scanning paths for 3s, 283s, 557s (seen Fig. 7 line 1, 2, 3). Herein, the laser beam center was located near the middle points of scanning line. It can be found that the highest temperature points were located at the center of laser beam. In fact, the peak temperature would locate behind the laser beam center if the scanning speed was fast. Temperature along scanning paths increases with time. Fig. 9b is the temperature along the depth at the highest temperature points. Peak temperature increases with time. Also for a constant depth, the temperature increases with time. It also can be drawn from the curves that whether the metallurgical bonding are formed, and how deep the melting pool is.

In order to achieve higher laser sintering quality sintered layer should be uniformly melted on the substrate, meanwhile substrate should be minimally diffused to the sintered layer. Substrate should be melted only with small depth, just to make the metallurgical bonding. But it was difficult to achieve, because temperature of laser irradiated area goes higher, and the melting pool

becomes deeper due to the heat accumulation. One solution for this issue is assumption of temperature dependent for power absorption from laser which is absorption of higher laser power at the beginning of simulation and then adjusting the absorptivity based on surface temperature.

Fig. 9 Temperature field of multi-track laser sintering at different line

(a) Center line of laser scanning paths (b) In depth direction at highest temperature point

Due to lack of access to required computation power we were not able to implement this idea, but we examined the simulation by changing the laser power and keeping all other parameters fixed. 3 groups of parameters as shown in table 6, were used.

Table 6 Parameters for sets

parameter	set1	set2	set3
absorptivity of coating layer	0.8	0.8	0.8
laser power/W	60	80	100

Fig. 10 a-c are the sketch up of cross section at the points corresponding to 3s, 283s and 557s. The red color areas represent the melting part. Fig.11a was the simulation results of parameters set1, it can be found that there is no melting area at 3s, because the laser power was low. At 283s, the melting depth was only about 0.05mm, and the melting pool depth almost increases to 0.1mm at 557s. The depth of melting pool was still not enough at the first scan line on Fig. 10b. At 283s and 557s the melting pools become deep enough, due to higher laser intensity utilized. From Fig. 10c, it can be seen that the melting pools depth were all larger than 0.1mm, which provides the whole coating layer metallurgical bonded together with the substrate. However, the substrate was over melted, therefore degrades the quality of sintered layer, because substrate material was mixed with the coating layer. From these results, it is obvious that melting pool profiles expanded with scanning time. This originates from thermal accumulation of pre-scanning.

Table 7 indicates the depth of melting pool and width of metallurgical bonding at the points of 3s, 283s and 557s, simulated with parameter set2. The substrate melted at the first scanning, since the melting depth was not enough. At 283s and 557s, the metallurgical bonding were formed, however, the width was still inadequate. In order to improve the bonding, the step size or the scanning speed should decrease; the laser power should be increased.

Simulation results proved that using these parameters Sets, the thoroughly metallurgical bonding could not be obtained as well as minimum uniform melting of substrate. It can be improved by: a) scanning after the heat affected zone cools down. But it will decrease the efficiency drastically, b) adjusting the parameters, such as decreasing the laser scanning power after the sample heats up, or for preheated sample.

Fig. 10 Melting pool cross section of multi-track laser sintering

(a) Parameters Set1 (b) Parameters Set2 (c) Parameters Set3

Table 7 Melting pool dimension with the parameters set2

Position	Depth of melting pool	Width of melting pool on the substrate surface
3s	0.08	0.31
283s	0.11	0.50
557s	0.18	0.62

Fig. 11 Temperature of point 1, 2, 3 under different laser sintering parameters

(a)Set1, (b) Set2, (c) Set3

Fig. 11 shows the thermal cycle curves of points 1、2、3 (as shown in Fig. 7) under different laser sintering parameters. It can be found that the temperature-time curves of the points are serrated. When the laser passes the point, the temperature peak appears. For each curve, the heating rate is similar to cooling rate, because laser scanning is with slow speed.

It is mainly laser heating that causes the rapidly increase of temperature of these three points. The heating effect of laser beam decreases as it goes away. Also the cooling rate decreases, correspondingly because it is a natural cooling process. Minimum temperature for three points

increases due to thermal accumulation in the sample. It also can be observed from the curves that maximum temperature and melting pool size follow the same trend: Fig. 11 shows significant increase in maximum temperature.

4 Experiment results

In order to verify the reliability and accuracy of the simulation results, the single track laser sintering experiments were performed. Parameters used in laser sintering process were the same as referred in numerical simulation process. Fig. 12 demonstrates images of the samples. It can be seen that sintered tracks are different for laser power, high laser power results in wide track and thick melted layer. Table 8 content the measurement results of the thickness of melted material and width of metallurgical bonding at joint surface. They were measured on the middle cross section of each sample. 60W laser power was too small to melt the Ni powder, after laser sintering, no material was melted in the sintered area. It is consistent with the simulation result. Comparing the other results (under 80W and 100W) with simulation results, it can be found that the measured results depict slightly larger melting pool than simulation output. It is mainly due to simplified assumptions for the simulation, as well as complications accompanying the melting process which is difficult to predict. In fact, as shown in Fig.13 (for sample under 100W laser power) after cleaning there exists slight balling on sintered track, and the sintered material is not uniformly located on the substrate surface. It looks like there is a variation inherent in sintering process of composite layer. This creates significant variability in the measured results. But, generally the simulation outputs are consistent with overview of experimental results, which qualifies this simulation method to be used for prediction of temperature distribution in laser sintering process of Ni-Gr nanocomposites.

Fig. 12 Single track laser sintered Ni-Gr samples.

Fig. 13 Laser sintered line after cleaning the sample (100W).

Table 8 Experiment results under different laser power at middle of the laser scanning line (3.5s)

Experiment	Exp-P1	Exp-P2	Exp-P3
Laser power/W	60	80	100
Depth of melting pool/mm	0	0.09	0.105

Width of metallurgical bonding at joint surface/mm	0	0	0.08

5 Conclusions

Single-track and multi-track temperature distributions of laser sintering Ni-Gr nanocomposites were studied. Relevant factors, such as, composite coating layer properties, temperature related thermophysical parameters and latent heat of phase change; the FEA models were established with reasonable simplification. Firstly, single-track laser sintering process was simulated; the temperature field distribution, melting pool shape and size were investigated. Then, multi-track laser sintering process was studied. Similar to single-track simulation, the temperature field distribution, and measurements of melting pool shape and size were accomplished.

In addition, the effects of former scanning on later scanning were investigated, and the thermal accumulation effects were discussed. In order to verify simulation results, experiments were performed under the same laser sintering parameters. In sum, the following conclusions can be drawn:

- (1) Comparing simulation outputs with experiments results, it can be found that consideration of convection and radiation heat transfer, and phase transition, can give out reasonable results.
- (2) Temperature distribution of laser sintering can be obtained from the simulation and accordingly melting pool depth and the metallurgical bonding width can be determined.
- (3) In multi-track laser sintering process, the thermal accumulation effects will govern the sintering quality. Suggested improving methods are decreasing the laser powder after the first step of sintering and/ or preheating the sample.
- (4) The optimal laser sintering parameters can be predicted feasibly by simulation results.

Acknowledgements

GJC acknowledge the financial supported by US National Institute of Standard and Technology (NIST) and Office of Naval Research. ZH thanks support from Open Fund of Jiangsu Provincial Key Laboratory for Science and Technology of Photon Manufacturing (Jiangsu University GZ201301) and Colleges and Universities in Jiangsu Province plans to graduate research and innovation (CXLX13_168).

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