Numerical simulation of laser cladding AlCrCuFeNi2 high-entropy alloy coatings

Zhiling Zhang, Honggang Yang* and Yunxia Chen
Department of Mechanical Engineering, Shanghai Dianji University, Shanghai, 201306, China

*Corresponding author’s e-mail: yanghg@sdju.edu.cn

Abstract: Laser cladding technology is an advanced material surface modification technology, which has the advantages of good combination of coating and substrate, and environmental protection process. In this paper, for the laser cladding of AlCrCuFeNi2 high-entropy alloy coatings, the effects of different laser powers and scanning speeds on the temperature and velocity fields were analyzed by numerical simulation. In the early stage of laser cladding process, heat transfer is dominated by heat conduction, and in the middle and later stages, convection dominates. Compared with the scanning speed, the laser power has a greater influence on the temperature peak inside the molten pool. The research results can provide a reference for the optimization of process parameters of laser cladding high-entropy alloy coatings.

1. Introduction
Laser cladding uses a high-power density laser beam as a heat source, and scans the surface of the substrate according to a set path. The surface of the substrate is rapidly melted under the irradiation of the laser beam, and the molten powder and substrate flow and mix in the molten pool and solidify rapidly. A dense alloy coating is formed, and finally the purpose of optimizing the properties of the substrate is achieved[1-3]. The laser cladding process involves many physical phenomena, such as laser-powder interaction, heat and mass transfer and fluid flow. It is very difficult to study the forming mechanism of cladding layer only by experimental means, and it has the disadvantages of low efficiency, long cycle and high cost[4]. Therefore, the use of numerical simulation methods for research is an efficient and meaningful means.

Khamidullin et al.[5] addressed the gas powder flow from a coaxial nozzle as a mixture of two interpenetrating fluids, and used the phase field method to simulate the phase transition process in two-dimensional and three-dimensional spaces. The results show that the two-dimensional method is effective in the simulation. It has good applicability under low scanning speed and low powder feeding speed. Wu et al. [6] simulated two process modes of unidirectional scanning and reciprocating scanning based on the finite element method, and the results show that the heat accumulation under the reciprocating scanning path is greater than that under the unidirectional scanning path. Zhang et al. [7] simulated the temperature field during the laser cladding process by using the life-death unit technology. The results showed that the larger the cladding thickness and the fewer layers, the lower the temperature peak and the smaller the temperature variation during the processing. Huang et al. [8] established a multiphysics numerical model considering the interaction process of laser-powder-melt pool. The Lagrangian particle method is used to solve the process of powder transportation a, and the interaction between powder and melt pool and its flow solidification process are further combined with the finite
volume method and the fluid volume method. The morphology and size of the single-pass cladding layer under different process parameters are predicted, and the change trend of the cladding layer morphology is analyzed. Wang et al.\cite{9} established the temperature field model of laser secondary scanning, extracted the thermal cycle curve of the key nodes of the cladding layer, combined with the experimental verification, and analyzed the influence of peak temperature and heat dissipation capacity on the change of coating structure growth. The results show that with the increase of the laser secondary scanning power, the grains of the cladding layer tend to grow thicker and larger, and when the secondary scanning power is too large, the melting area of the substrate will be enlarged and the dilution rate of the coating will be increased.

High-entropy alloys are generally formed by alloying no less than five metal elements in an equimolar ratio or approximately equimolar ratio, and have excellent properties such as high strength, high hardness, and excellent corrosion resistance\cite{10}. At present, most of the research on laser cladding high-entropy alloy coatings is carried out experimentally. In this paper, a simulation analysis of laser cladding AlCrCuFeNi2 high-entropy alloy coatings on the surface of Ti6Al4V titanium alloy is constructed based on the finite element method. The distribution of temperature and velocity and influence of different process parameters on the distribution are investigated.

2. Numerical simulation model

2.1. Model Assumptions

To simplify the model, the following assumptions are made:

- The liquid metal in the molten pool is a Newtonian, incompressible, laminar fluid.
- The laser heat flow is assumed to be Gaussian distribution.
- The powder falls into the molten pool area and is immediately melted.
- The energy decay of the laser beam through the powder flow is ignored.

2.2. Governing Equations

The continuity equation, the momentum conservation equation, and the energy equation are as follows:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]  
(1)

\[ \frac{\partial \rho}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \cdot \mathbf{u} = \nabla \cdot [-\rho \mathbf{I} + \mu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] - K_0 \frac{(1-f)}{f_0^3 + B} \]  
(2)

\[ \rho c_p (\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T) = \nabla \cdot (k \nabla T) - \frac{\partial H}{\partial t} - \rho \mathbf{u} \cdot \nabla H \]  
(3)

Among them, \( \rho, t, \mathbf{u} \) represent the density, flow time, velocity of the liquid in the molten pool, respectively. \( \mu \) represents the viscosity, \( p \) represents the pressure, \( T \) represents the temperature, \( c_p \) represents the specific heat, and \( k \) represents the thermal conductivity. In equation (3), \( H \) is the latent enthalpy of fusion:

\[ \Delta H = L f_l \]  
(4)

Where \( f_l \) represents the liquid mass fraction.

2.3. Boundaries and initial conditions

The mathematical model of the laser heat source is as follows:

\[ q = \frac{2Q \eta_l}{\pi r_b^2} \exp \left( -\frac{2((x-V_s y)^2 + y^2)}{r_b^2} \right) \]  
(5)

Among them, \( Q \) represents the laser power, \( r_b \) represents the radius of the laser beam, \( x \) and \( y \) represents the abscissa and ordinate of the laser heat source, respectively, and \( V_s \) represents the scanning speed. \( \eta_l \) represents the absorption rate of laser energy.

The motion of the molten pool surface was simulated using a moving mesh based on the Arbitrary Lagrangian-Eulerian method (ALE)\cite{11}, and the interface moving velocity due to powder addition.\cite{12}:
2.4. Model parameters

A symmetric model for numerical simulation is established. The substrate is Ti6Al4V, with a length, width and height of 8mm, 3mm, and 2.5mm, respectively. The powder is AlCrCuFeNi2 high-entropy alloy. The mass components of the substrate and powder are shown in Table 1. Table 2 shows the thermal physical properties of the substrate and powder, which are obtained by calculation and interpolation.

During the laser cladding process, the spot radius is 1.5mm, the powder feeding rate is 5 g/min, the convective heat transfer coefficient is set to 100, the powder capture efficiency is 0.9, the diffraction rate is 0.8, and the energy absorption rate is 0.3.

$$V_s = \frac{2m_f \eta_m}{\rho_m \pi r_p^2} \exp\left(-\frac{2((x-V_t t)^2 + y^2)}{r_p^2}\right)$$

Among them, $m_f$ represents the powder feeding rate, $\eta_m$ represents the powder capture efficiency, $\rho_m$ represents the powder density, and $r_p$ represents the powder feeding radius.

### Table 1. mass fraction(wt%)

| Material    | Ni  | Fe  | Cr  | Cu  | Al  | Ti  | V   | C   | O   | N   |
|-------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Ti6Al4V     | -   | 0.18| -   | -   | 6.51| Bal | 4.13| 0.02| 0.185| 0.01|
| AlxCrCuFeNi2| Bal | 17.7| 16.4| 20.2| 8.5 | -   | -   | -   | -   | -   |

### Table 2. Thermal physical properties of Ti6Al4V and AlCrCuFeNi2

| T/K     | $\rho/\text{kg} \cdot \text{m}^{-3}$ | $k/\text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$ | $c_p/\text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$ |
|---------|--------------------------------------|-----------------------------------------------------|-----------------------------------------------------|
| Ti6Al4V | AlCrCuFeNi2                          | Ti6Al4V                                             | AlCrCuFeNi2                                         |
| 873.15  | 4333.81                              | 7219.79                                             | 16.52                                               |
| 973.15  | 4325.23                              | 7172.66                                             | 17.35                                               |
| 1073.15 | 4311.52                              | 7030.63                                             | 19.13                                               |
| 1173.15 | 4304.62                              | 6977.65                                             | 21.33                                               |
| 1273.15 | 4313.72                              | 6910.73                                             | 24.28                                               |
| 1373.15 | 4295.91                              | 6813.71                                             | 25.92                                               |
| 1473.15 | 4276.89                              | 6566.19                                             | 27.55                                               |
| 1573.15 | 4257.16                              | 6396.12                                             | 29.17                                               |
| 1673.15 | 4236.74                              | 6320.36                                             | 30.80                                               |
| 1773.15 | 4215.63                              | 6242.21                                             | 32.42                                               |

3. Results and Discussion

3.1. Heat transfer inside the molten pool

The temperature field and velocity field were simulated with a laser power of 1800 W and a scanning speed of 12 mm/s. Figure 1 shows the distribution of temperature at different times. In the initial stage of the laser cladding process, the temperature of the workpiece region irradiated by the laser beam increases rapidly, and when the highest temperature reaches melting point of the workpiece, solid-liquid phase transition begins to appear and a molten pool is formed. The heat transfer is mainly carried out by convection and heat conduction, and the importance of convection to heat transfer can be measured by Peclet number.

Figure 2 shows distribution of velocity at different times. In the early stage (t=0.05 s), the liquid flow rate is very small, and the maximum flow rate is 3.56×10^{-3} m/s. At this time, the calculated Peclet number is only 0.65, indicating that heat conduction is dominant in the heat transfer inside the molten pool. As cladding process goes on, the molten pool continues to expand and the convection continues to increase. At t=0.1 s, the maximum flow velocity on the molten pool surface has reached 0.38 m/s, and the calculated Peclet number is 96, which indicates that convection has dominated the heat transfer.
3.2. Influence of different power on heat transfer inside the molten pool
Figure 3 shows the maximum temperature of the molten pool at each moment when the scanning speed is 12 mm/s and the laser power is 1500 W, 1800 W and 2000 W, respectively, and the temperature gradually becomes stable after rising rapidly in the initial stage. The higher the laser power, the faster the temperature rises and reaches a steady state. At 1800 W and 2000 W power, the maximum temperature has little difference after leveling off, both around 2500 K. The maximum temperature at the same time at 1500 W power is significantly lower, around 2375 K. Figure 4 shows the maximum temperature gradient in the directions of X, Y, and Z at each moment at 2 KW laser power and 12 mm/s scanning speed. It can be seen that the temperature gradient peak value of the workpiece in the height Z direction is always greater than the temperature gradient peak value in the horizontal direction at each moment, indicating that the heat dissipation speed of the normal direction of the solid-liquid interface is the fastest.
3.3. Influence of different scanning speeds on heat transfer inside the molten pool

Figure 5 shows the maximum temperature at each moment when the laser power is 2000 W and the scanning speed is 8 mm/s, 10 mm/s and 12 mm/s respectively, indicating that different scanning speeds have little effect on the temperature peak. Figure 6 shows the maximum temperature gradient in the directions of X, Y, and Z at each moment at 2 KW laser power and 8 mm/s scanning speed. The temperature gradient of the workpiece in the Z direction is also significantly greater than the temperature gradient in the X and Y directions. Comparing Figures 4 and 6, it can be found that the greater the scanning speed, the greater the Z-direction temperature gradient after stabilization. This is mainly because the slower the scanning speed is, the more heat is accumulated per unit time, causing the heat dissipation speed is relatively small. So the heat dissipation speed when the scanning speed is 12 mm/s is faster than that when the scanning speed is 8 mm/s, that is, the temperature gradient becomes greater.
Fig 5. Highest temperature in the molten pool at different times under different scanning speeds

Fig 6. Maximum temperature gradient in X,Y,Z direction at different times (scan speed 8mm/s)

4. Conclusion
(1) The numerical simulation of laser cladding of AlCrCuFeNi2 high-entropy alloy was carried out with titanium alloy as the base material, and the distribution law of temperature field and velocity field was obtained. With the increase of energy, the convection is continuously enhanced, and the convection is dominant in the heat transfer process in the middle and late stages.

(2) By comparing the internal temperature peaks of the molten pool under different laser powers and scanning speeds, it is found that the laser power has a greater impact on the temperature field. Compared with power, the influence of scanning speed on the temperature field is small, and there is little difference in the maximum temperature inside the molten pool at different times under different scanning speeds.

(3) By comparing the peak values of temperature gradients in the three dimensions under different laser powers and scanning speeds, it is found that the temperature gradient in the height Z direction is always the largest, that is, the heat dissipation in the normal direction of the solid-liquid interface is the fastest. And the greater the scanning speed, the larger the temperature gradient.

references:
[1] Zhang, J., Shi, S., Gong, Y., et al. (2020) Research progress of laser cladding technology. Surface Technology, 49: 1-11.
[2] Li, C., Yu, Z., Gao, J., et al. (2019) Multi-field coupled numerical simulation and experiment of laser cladding process heat-elastic-plastic-flow. China Surface Engineering, 32:124-134.
[3] Hu, D., Liu, Y., Chen, H., et al. (2021) Microstructure and properties of Ni-based WC coatings by laser cladding on Q960E steel. China Laser, 48: 239-245.
[4] Huang, C., Chen, J., Zhu, Y., et al. (2021) Powder-scale multiphysics numerical simulation of laser cladding.
directed energy deposition. Chinese Journal of Mechanics, 53: 3240-3251.

[5] Khamidullin, B.A., Tsivilskiy, I.V., Gorunov, A.I., et al. (2018) Modeling of the effect of powder parameters on laser cladding using coaxial nozzle. Surface & Coatings Technology, 258: 898–907.

[6] Wu, M., Ma, P., Bai, W., et al. (2021) Numerical simulation of temperature field-stress field during 316L/AISI304 laser cladding process under different scanning strategies. China Laser, 48:18-29.

[7] Zhang, Z., Ge, P. (2016) Finite Element Simulation of Laser Additive Manufacturing Process. Mechanical Research and Application, 29:136-139.

[8] Huang, C., Chen, J., Zhu, Y., et al. (2021) Powder-scale multiphysics numerical simulation of laser directed energy deposition. Acta Mechanica Sinica, 53: 3240-3251.

[9] Wang, W., Sun, W., Zhang, Z., et al. (2022) Study on Microstructure Evolution and Numerical Simulation of Laser Secondary Scanning Cladding Coatings. Materials Review, 36: 129-135.

[10] Di, Y., Liu, H., Zhang, X., et al. (2021) Friction, wear and high temperature oxidation resistance of AlCoCrFeMoVTi high-entropy alloy coatings by laser cladding on titanium alloy surfaces. Rare Metal Materials and Engineering, 50:2883-2891.

[11] Chan, R.K.C. (1975) A generalized arbitrary Lagrangian–Eulerian method for incompressible flows with sharp interfaces. Comput. Phys, 17:311–331.

[12] Morville, S., Carin, M., Peyre, P., et al. (2012) 2D longitudinal modeling of heat transfer and fluid flow during multilayered direct laser metal deposition process. Laser Appl, 24: 32-38.