

APPLICATION OF ENTHALPY METHOD FOR MOVING BOUNDARY PROBLEM IN LASER SURFACE MELTING*

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ABSTRACT A numerical analysis was carried out to study the moving boundary problem in the physical process of pulsed Nd-YAG laser surface melting prior to vaporization. The enthalpy method was applied to solve this two-phase axisymmetrical melting problem. Computational results of temperature fields were obtained, which provide useful information to practical laser treatment processing. The validity of enthalpy method in solving such problems is presented.

KEY WORDS enthalpy method, pulsed Nd-YAG laser, Stefan problem, temperature field, latent heat of fusion

1. INTRODUCTION

In the field of material processing, laser as a new-type clean, high-efficiency heat source is used in metallic material surface treatment. Various kinds of laser treatment techniques have attracted much attention for their applicability to the treatment of complex workpieces, flexible processing systems, etc. In recent years, the laser-texturing technique via Nd-YAG laser has been developed and successfully used in cold roll for steel sheet forming. With this technique, the mechanical properties of the laser-textured cold-roll are greatly improved and the coating quality of steel sheet is upgraded^[1-3], although the Nd-YAG laser has the disadvantage of small power capacity. In order to fully explore its potentiality in improving mechanical properties, such as wearing resistance, fatigue life, etc., engineers need more knowledge about laser/material interaction. Parameters optimization and active process design are expected.

As illustrated in Fig. 1, the fundamental process of material melting under Nd-YAG irradiation usually consists of four stages. Because both the duration (10^{-9} — 10^{-5} s) and the characteristic size (beam radius $\approx 10^{-5}$ m) are very small, numerical simulation becomes a possible method for studying this problem. This paper aims at the numerical analysis of temperature field when Nd-YAG laser is irradiated on the metallic material surface. The enthalpy method is adopted to solve this

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moving boundary problem. Numerical simulation results of the melting process are obtained, which provide new reference to the Nd-YAG laser surface treatment.

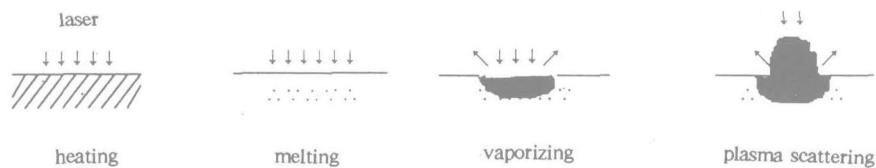


Fig. 1 Schematic of laser/material interaction.

II. MODELING OF THE PROBLEM

During the irradiation of laser beam onto the surface of a metallic workpiece, a portion of laser energy will be absorbed by the surface layer and converted into heat. It was estimated that such a transformation occurs in the layer $0.1\ \mu\text{m}$ thick from surface. Thereafter, the energy is transmitted into the substrate in the form of heat and results in temperature rising. For alloys, three different zones will co-exist, i. e. the mushy zone, solid zone and liquid zone, as shown in Fig. 2.

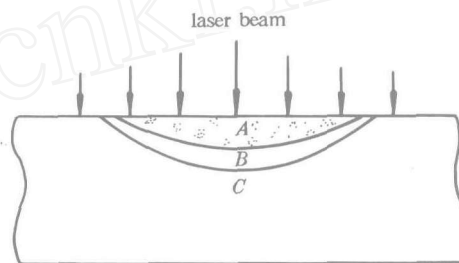


Fig. 2 Physical graph of partly molten alloy workpiece.
(A: liquid zone; B: mushy zone; C: solid zone)

In the melting process of material surface layer, the positions of interfaces between liquid/mushy zone and solid/mushy zone may change with time. A problem relating to such moving boundaries is called Stefan problem^[4-6]. If we make the following assumptions; (1) the energy density profile of the laser beam is of Gaussian type, and (2) heat affected zone is far smaller than the characteristic size of the workpiece, then we can establish an axisymmetrical heat conduction model in semi-infinite space. In addition, for simplicity

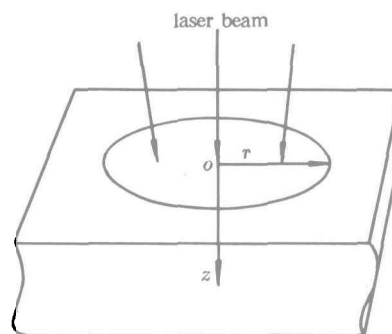


Fig. 3 Axisymmetrical co-ordinate system adopted.

in calculation, we assume that the material properties of mass density ρ , absorptivity A , specific heat c_p and thermal diffusivity a are of the same value in the solid and liquid states. Such an assumption will not affect the tendency of simulation results. In this model, the mushy zone is considered in the simulation of the two-phase moving boundary problem. Thus, the temperature field is readily obtained, with the effect of latent heat taken into consideration. With the axisymmetrical

co-ordinate system shown in Fig. 3, the equilibrium equations are:

$$\begin{cases} \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) + \frac{\partial^2 u}{\partial z^2} - \frac{1}{a} \frac{\partial u}{\partial t} = 0 & \text{for } g(\xi, \eta, t) \geq 0, \text{ i. e. , } u \geq T_l \\ \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) + \frac{\partial^2 u}{\partial z^2} - \frac{1}{a} \frac{\partial u}{\partial t} = 0 & \text{for } g(\xi, \eta, t) \leq 0, \text{ i. e. , } u \leq T_s \\ \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u''}{\partial r} \right) + \frac{\partial^2 u''}{\partial z^2} - \frac{\rho}{K_m} \frac{\partial Q_L(u)}{\partial t} - \frac{1}{a} \frac{\partial u''}{\partial t} = 0 & \text{for } g(\xi, \eta, t) \leq 0, g(\xi, \eta, t) \geq 0, \\ & \text{i. e. , } T_s \leq u'' \leq T_l \end{cases} \quad (1)$$

where u is temperature; t is time variable; the letters l , m , s in subscript and superscript represent the quantities in the liquid zone, mushy zone and solid zone respectively; T_0 is the ambient temperature; T_s is the solid temperature while T_l is the liquid temperature; $g(\xi, \eta, t) = 0$ and $g'(\xi, \eta, t) = 0$ are mathematical descriptions of the positions of interfaces of liquid/mushy zones and mushy/solid zones, denoted by A/B and B/C in Fig. 2.

The fixed boundary conditions and initial conditions are:

$$\frac{\partial u(r, 0, t)}{\partial z} = -\frac{q(r)}{K_s} \quad (2)$$

$$\begin{cases} \frac{\partial u(\infty, z, t)}{\partial r} = \frac{\partial u(r, \infty, t)}{\partial z} = 0 \\ u(\infty, z, t) = u(r, \infty, t) = T_0 \end{cases} \quad (3)$$

$$u(0, 0, 0) = T_s, \quad u(r, z, 0) = f(r, z), \quad g(r, 0, 0) = 0 \quad (4)$$

where $q(r)$ is the laser energy density on the surface, representing energy input, and $f(r, z)$ is the temperature distribution at the time the molten pool begins to be shaped, i. e. when the central point of the laser spot is at the solid temperature T_s after laser radiation. This model description denotes the time as initial time since before this time there is no liquid zone other than that in the moving boundary problem.

In particular, on the boundaries of the mushy zone, the following equations should be satisfied:

$$\begin{cases} K_m \frac{\partial u''(\xi'', \eta'', t)}{\partial n} - K_l \frac{\partial u'(\xi', \eta', t)}{\partial n} = Q_L v_n(\xi', \eta', t) \rho \\ K_m \frac{\partial u''(\xi'', \eta'', t)}{\partial n} - K_s \frac{\partial u(\xi', \eta', t)}{\partial n} = 0 \\ u(\xi', \eta', t) = T_l, \quad u(\xi'', \eta'', t) = T_s \end{cases} \quad (5)$$

in which Q_L is the latent heat of fusion, $v_n(\xi', \eta', t)$ is the mass velocity normal to the moving boundary $g'(\xi', \eta', t) = 0$.

Calculation based on the above expressions will face two main difficulties. First, the three zones are of different phases, and the nonlinearity of temperature gradient jump causes difficulty in analytical or numerical treatment of the problem. Second, the governing equations and moving boundaries are coupled since v_n is unknown. Because of these factors, the conventional methods of analysis and calculation are virtually invalid.

III. COMPUTATIONAL THEORY OF ENTHALPY METHOD

In the past two decades, numerical calculation methods have been developed for the solution of Stefan problem. Typical numerical methods include Method of Lines^[4-7], Variational Inequalities Method^[4-6], Isotherm Migration Method^[5-8] and Enthalpy Method^[5-6,8-15]. In the present situation, high energy-density pulsed laser irradiation may result in large temperature gradient within the surface layer. This is a great challenge to researchers in choosing a valid calculating method. If we consider that the alloy is not of a single molten temperature like a pure metal, but that a mushy zone exists, the enthalpy method may be the best choice.

First, we introduce the concept of enthalpy:

$$H(u) = \begin{cases} \int_{T_m-\epsilon}^u \rho(\theta)c_p(\theta)d\theta, & \text{for } u \leq T_m - \epsilon \\ \frac{\rho Q_L}{2\epsilon}(u - T_m + \epsilon), & \text{for } T_m - \epsilon \leq u \leq T_m + \epsilon \\ \int_{T_m+\epsilon}^u \rho(\theta)c_p(\theta)d\theta + \rho Q_L, & \text{for } u \geq T_m + \epsilon \end{cases} \quad (6)$$

where $T_m = T_S + (T_L - T_S)/2$ and $\epsilon = (T_L - T_S)/2$, which is the half width of mushy zone. Thereby, function $H(u)$ is continuous in all the three zones, which helps to overcome the difficulty due to temperature gradient jump in the calculation of the equation group (1-4).

To simplify nonlinearity and expression, we adopt Kirchhoff transformation

$$\psi = \int^u K(\zeta)d\zeta \quad (7)$$

where $K(\zeta)$ is conductivity. Then, the problem described by Eqs. (1-4) can be concisely expressed as:

$$\frac{\partial H}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \psi}{\partial r} \right) + \frac{\partial^2 \psi}{\partial z^2} \quad (8)$$

$$\frac{\partial \psi(r, 0, t)}{\partial z} = q(r) \quad (9)$$

$$H(r, z, 0) = \rho c(T_0 - T_m + \epsilon), \quad \psi(r, z, 0) = K T_0 \quad (10)$$

$$\frac{\partial \psi(\infty, z, t)}{\partial r} = \frac{\partial \psi(r, \infty, t)}{\partial z} = 0 \quad (11)$$

$$\psi(\infty, z, t) = \psi(r, \infty, t) = 0 \quad (12)$$

where the moving boundary condition(Eq. (5)) is no longer present in the new model description. Compared with (1-5), the decoupled method expressed by Eqs. (8-12) has avoided the difficulty due to temperature gradient jump by the existence of latent heat. Thus, in the calculation of H and ψ field, whether the domain is in solid zone, mushy zone or liquid zone is not important. In this calculation, enthalpy is directly related in addition to the temperature variable. An explicit numerical calculation procedure then can be produced: (1) at time step $n+1$, calculating new H field by using discretized Eq. (8) from old ψ field; (2) calculating new ψ field from H field by Eq. (6); and (3) calculating ψ on boundaries according to Eqs. (10-12).

When the above calculations in each time step are completed, based on Eq. (6), the positions of every zone can be determined and the temperature field can be worked out. Thus, the calculation

in the whole physical domain can be realized. From the basic equations and the calculation scheme of the enthalpy method, numerical computation is carried out step by step to solve the coupling case between the governing equations and moving boundaries. Because with the enthalpy method a problem with nonlinearity coupling is transformed into a calculation scheme of fixed boundary problem, it is also classified as a fixed domain method^[5].

IV. CALCULATED RESULTS AND DISCUSSION

4.1 Temperature Field and Its Characteristics

Figure 4 shows the laser density profile adopted in our calculation which is of a Gaussian type. Figure 5 shows the profile of the general molten pool calculated. The temperature evolution graph when a metallic alloy is heated by pulsed Nd-YAG laser is illustrated in Fig. 6. It is obvious that the temperature of alloy surface will quickly rise to a certain level. We can also see that the aspect ratios of radius to depth of isotherms, ω , decrease with the advance of time scale, indicating that the isotherms develop faster in the depth direction than that in radial one and the mushy zone is so narrow that it cannot be distinguished clearly.

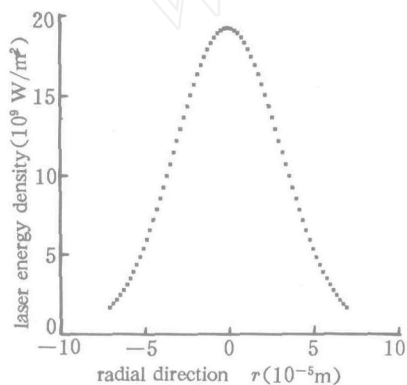


Fig. 4 Energy density of Nd-YAG laser in the calculation.

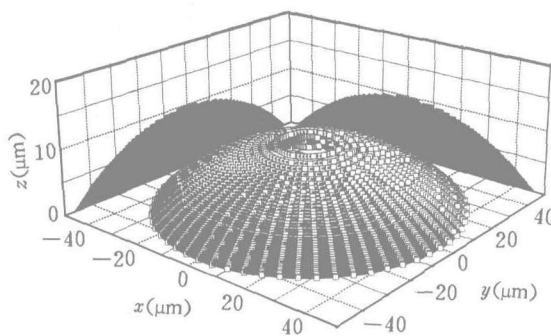


Fig. 5 Shape of molten zone at the time when vaporizing begins.

For any two neighboring isotherms with the same temperature difference, the smaller the distance between them, the greater the temperature gradient will be. Therefore, Fig. 6 also shows the gradient characteristics of temperature field. Near the surface, the value of temperature gradient is large. The gradient decreases quickly with the increase of z . These plots also suggest that the temperature gradient field in the surface layer becomes more intense with the passage of time.

4.2 Evolution of Moving Boundary

Figure 7 illustrates the temporal evolution of molten pool, in which t_v denotes the time when the central point on the surface begins to evaporate. From Fig. 7, it can be seen that the aspect ratio ω of molten pool decreases gradually. From the moment $t = 3.0 \times 10^{-6}$ s to $t = 7.0 \times 10^{-6}$ s, the aspect ratio of the latter case almost halves the value of the former case. This is helpful to understanding the influence of laser-texturing processing parameters on surface roughness after treatment.

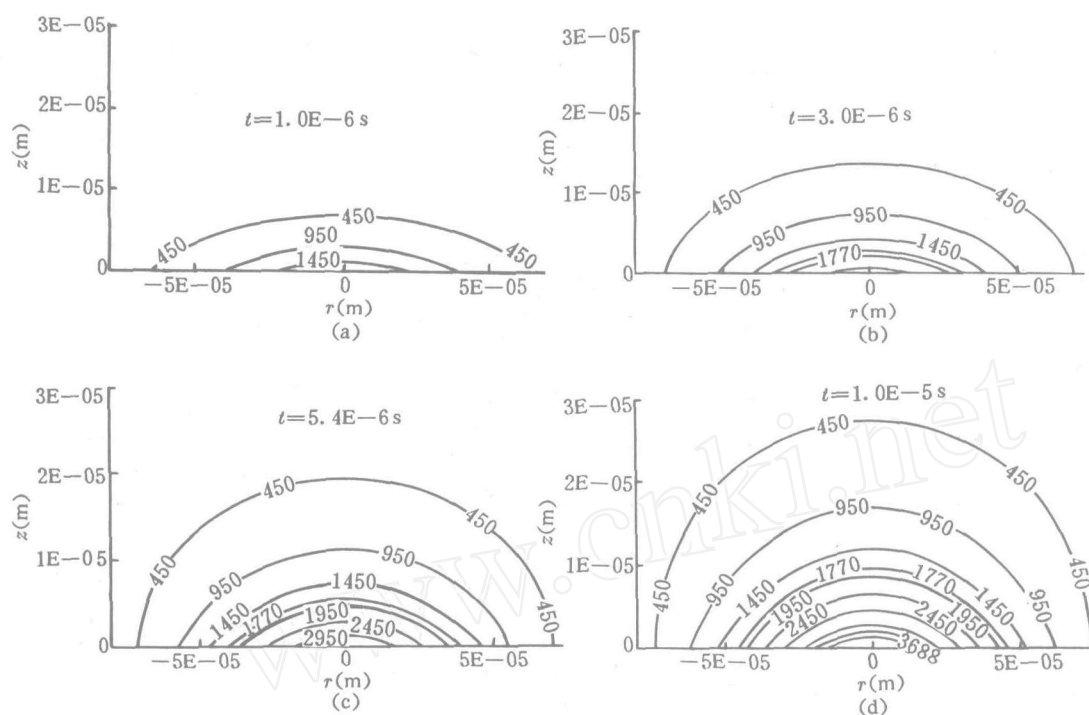


Fig. 6 Evolution of temperature field.

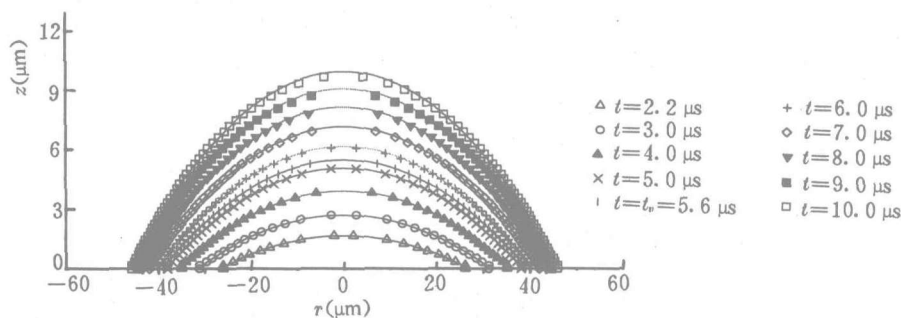


Fig. 7 Shape evolution of molten zone.

4.3 Effect of Latent Heat of Fusion

The advantage of the Stefan model is that it makes it easy to study the effect of the latent heat of fusion. As shown in Fig. 8, for cases in which latent heat Q_L is between 1.0 J/kg and $1.0 \times 10^4 \text{ J/kg}$, the results at $t = 5.5 \mu\text{s}$ are little different. However, the difference between the results for $Q_L = 2.9 \times 10^5 \text{ J/kg}$ (which is of the same magnitude with practical value) and the previous four cases is detectable, with the decrease of the aspect ratio by nearly 19%. While in Fig. 9, the difference between cases of $Q_L = 10.0 \text{ J/kg}$ and $Q_L = 2.9 \times 10^5 \text{ J/kg}$ is diminished. In other words, the influence of latent heat on the molten shape at the time of evaporation is small (nearly 5.3%). Since for all the vaporization time t_v longer than $5.5 \mu\text{s}$, we can argue that the latent heat will make

the aspect ratios decrease to some extent. On the other hand, it also causes the vaporization time to be prolonged. These two results indicate that the latent heat leads to prolonging the vaporization time t_v . This may further diminish the effect of latent heat on the difference of the aspect ratio. If the laser pulse is immediately terminated after vaporization begins, then the effect of the latent heat of fusion on the pulsed Nd-YAG laser-texturing processing may be ignored.

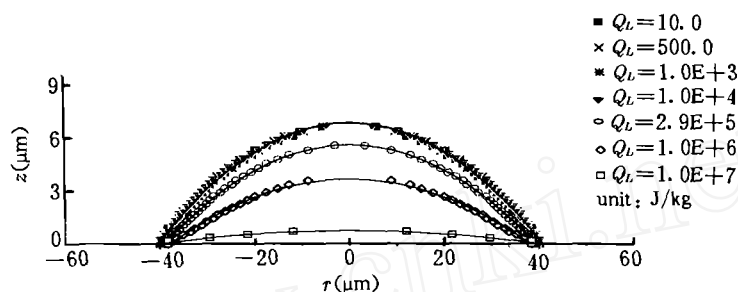


Fig. 8 Shapes of molten zone for different Q_L at 5.5 μ s.

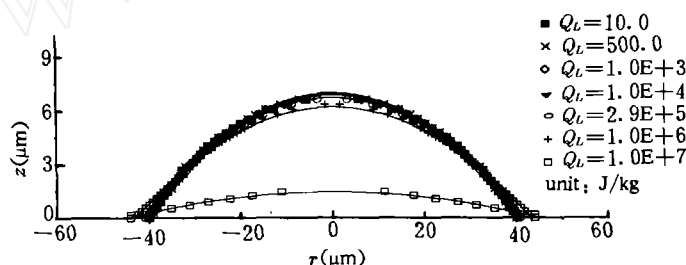


Fig. 9 Shapes of molten zone for different Q_L when the central point begins to evaporate.

V. CONCLUSIONS

In the present paper, a two-phase axisymmetrical thermodynamic model is established to calculate the temperature field induced by pulsed Nd-YAG laser irradiation on metallic materials. The enthalpy method is used in the calculation. The following conclusions are drawn.

(1) The temperature field and moving boundary positions of different lengths of duration are calculated. The results demonstrate that the enthalpy method is effective in researches on the moving boundary problem.

(2) The temperature field evolution is illustrated after studying the isotherms at different lengths of duration. During the evolution process of molten pool, the profile develops faster in the depth direction, while the temperature gradient concentrates on the centre of surface. The effect of the latent heat is considered, which makes aspect ratios increase and simultaneously delays the vaporization. However, the effect on the difference of the melting pool is very limited at time t_v .

(3) The moving boundary problem is a common problem in the nature. The process of laser melting is a special case. The application of the enthalpy method in the model calculation provides a

support to the understanding of the physical process in the laser/material interaction, which is useful to the future work on model improvement and material microstructure design.

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