Abstract: The aim of the research is to develop a simplified numerical model to predict the formation of the melt pool and the heat affected zone in single track laser alloying of C45 steel with NiCrBSi powder. The developed finite element model is based on the temperature field calculation using Fourier law. The unknown coefficients such as surface absorption coefficient, volumetric efficiency and beam distribution coefficients are set according to cross-section geometry data, obtained from laser alloying experiment. The Nd:YAG solid state laser was used to study the influence of power and scan feed rate on remelted cross-section area and microstructure. The calculated height and depth of melt pool and heat affected zone are in fairly good agreement with the experimental data. The presented numerical model requires further refinement in order to take into account the complex physical phenomena during laser melting and alloying.

Keywords: microstructure; C45 steel; laser alloying; laser cladding; NiCrBSi alloy; FEM.

1 Introduction

Laser alloying is a process of melting a material with a high-power laser and then adding other alloying elements into the molten pool or with pre-deposited layer (Toyserkani et al., 2005). Surface alloying and cladding when performed by a laser require minimal post-process re-machining of the surface and localised residual stresses (Grum and Žnidaršič, 2006). The laser alloying operating window is defined in terms of laser beam mode, power, spot diameter, scanning speed and powder feed rate. Only values of parameter setting within limited ranges can be applied to generate tracks meeting the geometrical requirements to produce crack and pore free coatings by overlapping single tracks (Felde et al., 2003). The thermo-kinetic laser powder deposition model coupling finite element heat transfer calculations with transformation kinetics and quantitative property–microstructure relationships was developed (Costa et al., 2005).

Surface alloying with a laser is similar to laser surface melting with the exception that another material is incorporated into the melt pool. In most modelling applications, assumptions must be made to reduce the complexity of the physical phenomena and to reduce the amount of pre- and post-processing time. The simplified temperature model for prediction of area cross-section in laser alloying where the heat input is presented using the idea of Guo and Kar (2000). The temperature field was calculated using the Fourier equation and under assumption that the molten pool is half-ellipsoid.
The numerical values were set according to experimental data to adjust the variables such as absorption coefficient, volumetric efficiency and the beam distribution coefficient.

2 Temperature field calculation

The numerical model is based on the calculation of the temperature in the substrate during the laser treatments. As a first approximation, the melt pool region as well as the heat affected zone is assumed to be in agreement with the peak temperatures obtained by the laser beam in the whole volume of the specimen. The temperature field was calculated by solving the Fourier formula,

\[ \rho C_p \frac{\partial T}{\partial t} + S \rho C_p \frac{\partial T}{\partial r} = \frac{\partial}{\partial r} \left( k \left( r \right) \frac{\partial T}{\partial r} \right) + Q \] (1)

where \( r \) vector denotes the local coordinates, \( T(r, t) \) is the temperature at any point of the substrate at a given time \( t \) to the velocity \( S \) of the laser beam moving above the fixed specimen, \( \rho \) is the density, \( C_p \) is the specific heat, \( k \) is the thermal conductivity and \( Q \) is the internal heat generation per unit time and unit volume. Equation (1) should be satisfied using the initial and boundary conditions illustrated in Figure 1.

Figure 1  Coordinate system used in laser alloying

At time \( t = 0 \), the substrate has a uniform temperature \( (T_0) \) throughout its volume,

\[ T(r,0) = T_0 \] (2)

The boundary conditions are:

\[ -k \left( T \right) \left( \frac{\partial T}{\partial r} \right) = h \left[ T - T_{\text{am}} \right] + e \sigma \left[ T^4 - T_{\text{am}}^4 \right] - q_s \] (3)

where \( h \) and \( e \) is the surface heat transfer coefficient and emissivity, respectively; \( \sigma \) is Stefan–Boltzmann constant and \( T_0 \) is the ambient temperature. The term \( q_s \) stands for the imposed heat flux onto the surface due to the laser beam. The heat input into the substrate due to the application of laser beam is considered in terms of surface heat flux (Guo and Kar, 2000) through the term \( q_s \) in equation until the top surface of substrate is below solidus temperature as
\[ q_r = \frac{P\eta_{\text{gauss}}d}{\pi R_{\text{eff}}^2} \exp\left( \frac{dR^2}{R_{\text{eff}}^2} \right) \]  

where \( P \) refers to beam power, \( \eta_{\text{gauss}} \) Gauss absorption coefficient, \( R_{\text{eff}} \) the effective radius of the laser beam and \( d \) is the distribution coefficient related to the pattern of the laser beam profile. As the substrate subsequently melts, the surface heat flux is replaced by a volumetric heat source expression for the portion of the molten substrate as

\[ \dot{Q} = \frac{6\sqrt{3}P\eta_{\text{vol}}}{\pi a^2 b} \exp\left( -\frac{3R^2}{a^2} - \frac{3\pi^2}{b^2} \right) \]

where

\[ a = R_{\text{eff}} \quad \text{for} \quad a \leq R_{\text{eff}} \]
\[ a = w_i \quad \text{for} \quad a > R_{\text{eff}} \]
\[ b = p_i \]

where \( w_i \) and \( p_i \) are instantaneous values of the computed width and penetration of the liquid pool, respectively, performed by the numerical calculations. The absorption coefficient of volumetric heat is \( \eta_{\text{vol}} \). The shape of the volumetric heat source was assumed to be an ellipsoid having axis \( a \) and \( b \). The heat input taken into account from equation (5) is applied directly into the melt pool volume through the term in equation (1).

3 Material and methods

3.1 Substrate and feedstock material

Experiments were carried out on substrate made from C45 steel (Mat. No. 1.0503). Figure 2(a) shows the network of ferrite–pearlite microstructure of substrate. Figure 2(b) shows nickel-based powder NiCrBSi, which was deposited in the molten pool during laser alloying through the nozzle of the laser head. Chemical compositions of the base and feedstock material are given in Table 1.

3.2 Specimen preparation

The specimens were laser alloyed at Bay Zoltán Institute in Budapest using the solid state Nd:YAG laser (Rofin), powder feeder system with carrier gas (argon), laser cladding head with circumferential arrangement of four nozzles injection. The laser track length was \( L = 50 \text{ mm} \) and the cross-section was examined on the plane with the offset of \( L/2 = 25 \text{ mm} \) from the laser start. The power levels were 1000, 1500, 2000 and 2500 W and scanning speeds were 400, 500, 600 and 700 mm/min.

Metallographic specimens were prepared following standard procedure and etched in nital solution. The cross-section images were acquired using optical microscope. The chemical analysis was carried out with JEOL JXA 8600 scanning electron microscope using energy dispersive spectroscopy.
4 Results and discussion

4.1 Temperature field

The temperature model has been discretised in the Comsol finite element model code. The real geometry of the substrate has been applied in the FEM model where the laser is scanned in x direction. Values of absorption coefficient, $\eta_{\text{guss}}$, volumetric efficiency $\eta_{\text{vol}}$ and beam distribution coefficient are considered to be 0.30, 0.35 and 3.0 to compute melt pool dimensions corresponding to all the experimental laser alloying conditions. In the model, we assumed the melting of the substrate occurs when the maximum temperature on the surface reaches liquidus point.

The calculated temperature during laser alloying with $P = 2500$ W and feed rate of 400 mm/min is shown in Figure 3. High, non-equilibrium heating rates move the transformation points $A_{c1}$ and $A_{c3}$ to higher temperature level. The short cooling time $t_{c/5}$ in a range from 0.5 to 0.8 s is a possible reason for generation of cracks in the melted zone (Figure 5(b)).

4.2 Experimental results

The geometry of cross-section was digitalised and the basic dimensions were taken into account: area cross-section, depth, width of melted and heat affected zone.

The relationship of the remelted area $A$ ($\text{mm}^2$), power ($P$) and scanning speed ($S$) is shown in Figure 4. The remelted area $A$ ($\text{mm}^2$) is increasing with power and decreasing with scanning speed $S$. Figure 5 shows the macro- and microstructure of alloyed region.
The calculated temperature during laser treatment at $P = 2500$ W and 400 mm/min: (a) isosurfaces after 3.25 seconds and (b) temperature as a function of time and depth (see online version for colours).

Figure 4 The remelted area as a function of power (see online version for colours)

The temperature transformation austenite (TTA) diagrams are used to predict the formation of austenite in the heated zone. The heating rate with laser is in a range of 1000°C/s, therefore the formation of austenite is at higher temperature than with very slow heating rate (in furnace). The temperature where the austenite starts depends on the heating rate. When the rate of heating increases, the austenite formation takes place at the higher temperature. The TTA diagram for C45 steel is presented in Figure 6. The energy dispersive spectroscopy linescan was made through each cross-section of metallographic specimen. The linescan values were averaged of each sample. The correlation of chemical composition and laser scanning parameters was not found when comparing the individual tracks made with different parameters. The average values, used for further analysis of alloyed material, show the average composition of 0.45% C, 5.4% Ni, 1.07% Mn, 0.96% Cr, 0.62% Si and 0.1% Mo. Figure 7 shows the TTA diagram for alloyed material. From the comparison of each diagram, it is evident that austenite on heating forms at lower temperature in the alloyed region than in the C45 steel.
Figure 5  Microstructure of alloyed zone and substrate: (a) macrograph of cross-section, specimen $P = 1000$ W, $v = 600$ mm/min; (b1) cracks in melted and alloyed zone; (b2) melted and alloyed zone and (c) transition microstructures in the heat affected zone (see online version for colours)
**Figure 6** Temperature transformation austenite (TTA) diagram for C45 composition (J MatPro) (see online version for colours)

**TTA diagram**

![TTA diagram for C45 composition](image)

*Initial microstructure: Normalised*

**Figure 7** Temperature transformation austenite (TTA) diagram for alloyed region averaged composition (J MatPro) (see online version for colours)

**TTA diagram**

![TTA diagram for alloyed region averaged composition](image)

*Initial microstructure: Quench tempered*
On macrograph of Figure 5, the decomposition of pearlite is visible on the elliptical $A_c1$ isotherm. We assume this temperature corresponds to around 830°C according to the TTA diagram for heating rate of 1000°C/s, Figure 6. Moreover, isothermal line, where ferrite grains disappear, indicates the $A_c3$ isotherm which is at around 930°C. The melted and alloyed region was subsequently subjected to high cooling rate; therefore, martensite was formed over the entire area. The 100% martensite also formed near the fusion line in the heat affected zone. High cooling rate (Figure 8) and the metallurgical effect of alloying contributed to hardness between 750 HV and 800 HV.

Figure 9 shows the comparison of remelted area cross-section of the model and experimental data. The lack of fit between the molten pool was observed at 1 and 1.5 kW. On the other hand, a good agreement between measured and predicted values is in the range from 2 kW to 2.5 kW. From the comparison, it is clear that the presented numerical model requires further refinement to order to take into account the complex physical phenomena during laser melting and alloying.

Figure 8  Continuous cooling diagram for C45 steel (see online version for colours)
5 Conclusions

The surface properties after laser alloying of C45 steel with NiCrBSi self-fluxing gas atomised powder were studied and the simplified temperature–time model was proposed. The real geometry of the substrate has been applied in the finite element model. The microstructure after melting and alloying is brittle and susceptible to hot cracking.

The predicted peak-temperature field is, in most cases, in a good agreement with the microstructural variation from cross-section images. However, in some cases, the width and the depth of the melted pool determined at real samples differ from the calculated ones. The reason of the discrepancy could be originated to the simplicity of the model which does not include several phenomena occur during the laser alloying of the substrate.

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