On the role of capillary and thermo capillary phenomena on microstructure at laser cladding

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Abstract. Laser cladding (LC) is a widely used additive manufacturing technology, but some shortcomings such as narrow processing window still limit it. The hydrodynamic model of LC for the calculation of the microstructure of built-up layer is developed considering contact angle of the melt with the substrate. The study of capillary phenomena, the influence of contact angle on characteristics of a built-up layer is held. The powder jet radius showed dissimilar response to the contact angle change depending on the comparison to the melt pool width. The track spreading due to contact angle change is shown to decrease the average crystalline size of the clad layer. The results provide the insight in to the LC technology can be used for the process optimization.

1. Introduction

Current metal-based additive manufacturing (AM) technologies suffer from a twofold drawback: (1) high production costs and (2) potential and sometimes unpredictable failure of the fabrication process. Nowadays, operators may need to do several attempts before succeeding, and most of the choices (e.g. part orientation, type and density of supports, ...) are done manually based on personal experience [1]. Laser cladding (LC) is a widely used AM technology, but some shortcomings such as narrow processing window still limit it. Direct numerical simulation (DNS) of heat-mass transfer during LC has proved to be a cost-effective method of searching for the optimal processing parameters which allows making a glance into this technology [2]. Application of the DNS to test the troublesome regions that could be identified at the process planning stage can boost the quality and flexibility of direct fabrication.

Nevertheless the fact that hydrodynamic phenomena after laser action is well studied, distinct convective effects after joint laser-powder action on substrate are poorly presented in the literature. The problem of taking into account the contact angle is solved in the certain cases of shock-capturing methods utilization [3], but in the LC models it is most often not taken into account [4]. In a broad sense this is not justified because the width of the melt spreading is of great importance for the basic parameters of the clad and the quality of the obtained layer. A large value of the contact angle, for example, leads to the formation of pores between successive tracks [5], and the specific form of the clad track and the penetration zone determines the quality of adhesion to the substrate [6].

The contact angle can be easily determined by track examination, so including the measured contact angle to the model can account for such factors that influence on it. The balance of a free interfacial energy in the multiphase system described by Young-Laplace equation gives the contact angle thus one can account not only for liquid melt surface tension, but for the interaction between three phases. Oxidation and roughness one of the main problems of LC influence contact angle, so these factors can be considered in the model with known contact angle.
A multiscale approach is used to simulate the microstructure at LC [7,8], where the temperature history calculated on a macroscale is used to calculate the microstructure evolution at the micro level. For the latter, the phase field method is often used, which provide the insight into the shape and size of the resulting grains. The need in the transfer function between scales makes derivation of fully self-consistent solution complicated in such models. It is often sufficient to know the average grain size of the resulting clad for real qualitative estimations of the microstructure, which opens the possibility of using simpler models [9].

The aim of this paper is to develop a coupled kinetic-hydrodynamic model of LC for the microstructure simulation of the clad layer, taking into account the known contact angle of the melt and the substrate. The kinetic process is described by Kolmogorov-Johnson–Mehl-Avrami (KJMA) equation with non-uniform nucleation and growth rates. The model allows investigating the spreading of molten powder onto a substrate with a different contact angle, to optimize and plan the LC process. The influence of contact angle on the main output parameters such as width, height and average crystalline size of the track is investigated. The model can account for oxidation, substrate roughness which is of great importance.

2. Numerical model

The developed model includes heat and mass transfer in a multiphase system: a gas - melt pool - solid substrate. The special attention is paid to the self-consistent solution of the system of equations, which simultaneously take into account the thermal conduction, convection, high-rate crystallization of the clad layer, and the motion of the interface accounting the known contact angle with the substrate. The hydrodynamic macromodel is described in details in our previous paper [10], the basic equations are similar to the published in recent years papers on LC [4,11]. The melted substrate is considered to catch 0.9 of the powder within the intersection with jet; contrariwise solid substrate is attributed to the particle skipping. The model for the microstructure simulation is considered by [9,12] and is not given here.

The main driving forces in the melt pool are surface thermo capillary forces [11]. Their competition with capillary forces determines the shape of the melt pool. These surface forces are introduced as volumetric sources in to the momentum equation in the three-phase media [13]:

\[ S_{surface} = (f_{capillary} + f_{marangoni}) \delta \]  

where \( \delta \) is the delta function, which can be calculated through the free surface capture function. Capillary forces are calculated by the formula:

\[ f_{capillary} = \sigma \kappa \]  

where \( \sigma \) is the surface tension, and \( \kappa \) is the curvature of the surface.

If \( n \) is the normal vector of the surface directed from the metal into the air, then for the curvature of the surface we have:

\[ \kappa = -\nabla \cdot n \]  

as

\[ n = \frac{\nabla \phi}{|\nabla \phi|} \]  

for the curvature of the surface we obtain the formula:

\[ \kappa = -\nabla \cdot n = -\nabla \cdot \frac{\nabla \phi}{|\nabla \phi|} \]  

where \( \phi \) - the free surface capture function. This formulation does not take into account the real contact angle of the liquid metal depending on substrate characteristics such as oxidation or surface roughness. There are many approaches to the modeling of the contact angle, but we assume that the track spreading is only occur (there is no reverse motion), and we use one fixed value of the contact angle. Considering this the z component of the normal of the free surface is not calculated by formula
(3), on the faces of the substrate, but is specified in accordance with the known (experimentally measured) value of the contact angle:

\[ n_z = -\cos(\theta) \]  \hspace{1cm} (6)

The curvature of the free surface is calculated through a modified normal and has increased values in the case of a contact angle other than the specified angle. Capillary forces that tend to decrease a curvature, adjust the free surface to the required contact angle.

The model is implemented in the open-source CFD library Openfoam version 2.3.x. The interFoam was chosen as a base solver and was adapted to our needs. PISO algorithm is used for the momentum and pressure equation consistence [14]. Free surface capturing function is implemented in Openfoam with the help of MULES algorithm [14]. The mesh is generated in blockMesh utility and is consisted of dense zone (11.5mm*2.85mm*2.5mm) with grid step of 0.05 mm in all directions and sparse regions outside of it. Only half of real space is modeled due to symmetry.

### Table 1. Thermal and kinetic parameters used for the simulation.

| Property                              | Parameter, units | Value | Property                              | Parameter, units | Value          |
|---------------------------------------|------------------|-------|---------------------------------------|------------------|----------------|
| Heat conductivity of solid metal      | \( \lambda_s \), W/(m*K) | 11    | Dynamic viscosity of metal            | \( \eta_m \), 10^-7 m^2/s | 6.872 [15]    |
| Heat conductivity of liquid metal     | \( \lambda_l \), W/(m*K) | 24    | Dynamic viscosity of air              | \( \eta_g \), 10^-5 m^2/s | 1.48           |
| Heat conductivity of air              | \( \lambda_g \), W/(m*K) | 0.03  | Surface tension                       | \( \sigma \), N/m | 1.778 [15]    |
| Density of metal                      | \( \rho_m \), kg/m³ | 7130  | Surface tension gradient              | \( \frac{\partial \sigma}{\partial T} \), mN/m*K | -0.38 [15]    |
| Density of air                        | \( \rho_g \), kg/m³ | 1     | Absorption coefficient                | \( \sigma_{abs} \) | 0.45           |
| Heat capacity of solid                | \( c_s \), J/(kg*K) | 419   | Latent heat capacity                  | \( L \), kJ/kg   | 227            |
| Heat capacity of liquid               | \( c_l \), J/(kg*K) | 754   | Number of sites                       | \( N_0 \), 10^14 cm² | 2.105          |
| Heat capacity of air                  | \( c_g \), J/(kg*K) | 1008  | Activation energy                     | \( E_a \), eV     | 0.5            |
| Solidus temperature                   | \( T_s \), K     | 1483  | Surface energy                        | \( \gamma \), erg/cm² | 70             |
| Liquidus temperature                  | \( T_l \), K     | 1583  | Lattice constant                      | \( d_0 \), 10^-8 cm | 3,524          |

![Figure 1](image1.png)

Figure 1. Distribution of crystallites in the cross-section of deposited droplets with different contact angle 10° (a) and 30° (b).

### 3. Results and discussion

The LC by a non-scanning beam with coaxial nickel powder feeding is simulated to study the influence of contact angle on the resulting microstructure. The substrates with a different wetting angle were used for that purpose. The used thermal and kinetic parameters are listed in table 1. The powder is fed (m = 50g / min, Rjet = 2mm) together with laser radiation (P = 1.5kW, Rbeam = 2mm) on a cold substrate for 50ms forming a single drop. Then laser radiation goes off, the drop cools down and crystallization occur. Figure 1 shows a typical picture of the crystalline distribution in the cross
section for drops with a contact angle of 10° (left) and 30° (right). Here and further, color shows the spatial distribution of crystallites, the white line is the boundary of the free surface, and the red line limits the crystallization zone. In the lower left corner of the figure, the average cross-sectional size of the crystallites is indicated.

The boundary of crystallization zone is deformed due to the influence of hydrodynamic flow. The central zone has higher crystalline size comparing to the peripheral area. The convection is most active at the beginning of the crystallization process when the droplet has the most temperature gradient. Then temperature gradient reduces and the fluid flow does not play the main role in the heat dissipation. It can be seen that the droplet, which has spread more along the substrate, has a somewhat smaller height and the average crystalline size. This is due to the different cooling rate of the investigated droplets. The heat transfer to the substrate is weaker for the concentrated droplet, due to the smaller contact area.

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### Table 2. Processing parameters.

| Notation of the set of parameters | highSpeed | lowSpeed |
|-----------------------------------|-----------|----------|
| $P$, W                            | 640       | 400      |
| $V_{\text{scan}}$, mm/s           | 50        | 20       |
| $\dot{m}$, g/min                  | 10        | 4        |
| $R_{\text{beam}}$, mm             | 1         | 1        |
| $R_{\text{jet}}$, mm              | 0.5       | 0.5, 1   |
| $\theta$, °                       | 10°-30°   | 10°-30°  |

Further, the effect of the contact angle on the geometric parameters of a single clad track, as well as its microstructure, was investigated. For this purpose, numerical calculations of LC on a massive substrate with different powder flow parameters for two scanning speeds were performed. The process parameters are given in Table 2. For simplicity, it is assumed that the powder flow has a uniform distribution. The powder is fed at the temperature $T_{\text{powder}} = 1000K$ coaxially with the laser beam, which has a topHat distribution. The used sets of parameters have the same mass per unit surface, but a different power density and are selected in such a way to obtain tracks of the same geometric dimensions at different scanning speeds.

### Table 3. The results of the simulation.

| Jet radius, mm | 1 (“wide”) | 0.5 (“narrow”) | 1 | 0.5 |
|----------------|------------|----------------|---|-----|
| Known contact angle | 10° | 30° | 10° | 30° | 10° | 30° | 30° |
| Track half width, mm | 0.99        | 0.87          | 1.02 | 0.89 | 1.017 | 0.907 | 1.03 | 0.922 |
| Track height, mm   | 0.271      | 0.288         | 0.293 | 0.334 | 0.248 | 0.247 | 0.297 | 0.331 |
| Catchment efficiency | 0.91       | 0.8           | 1 | 1 | 0.88 | 0.79 | 1 | 1 |
| Maximum flow rate, m/s | 0.54 | 0.63 | 0.61 | 0.609 | 0.564 | 0.67 | 0.702 | 0.69 |
| Maximum temperature, K | 1908 | 1959 | 1932 | 1931 | 2020 | 2062 | 2071 | 2069 |

Table 3 shows the output parameters of the cladded tracks for investigated sets. At high scanning speed, the catchment efficiency is lower, which leads to a different behavior of some output parameters compared to a low speed. We use here the notation “wide” and “narrow” powder jet comparing it to the melt pool. The results for a narrow and wide powder jet have qualitative difference. The output parameters of LC with different contact angle are compared for investigated processing parameters. The maximum flow rate is approximately 0.5 m/s and grows with the maximum temperature increase. The “highspeed” set of parameters showed higher maximum temperature due to the increased laser power.
Figures 2 a, b show a comparison of the cross sections of the tracks in the case of a wide powder jet for two values of the scanning speed. A high scanning speed (Figure 2 a) corresponds to high mismatch of melt pool and powder jet which results in a low catchment efficiency (see table 3). A complete intersection with the powder jet is still not reached at low speed (table 3). The lag to the powder jet is lower with scanning speed decrease, that’s why the height is slightly higher at low speed (Fig. 2 b). The track is spreading transversely to the scanning direction on more wettable substrate thereby capturing an additional amount of powder. The height of the track remains constant due to the fact that spreading does not increase the powder jet – melt pool intersection in the front direction.

Figures 2 c, d show a comparison of track profiles the case of a narrow powder jet, and the entire powder fed is always captured. In this case, a decrease in the contact angle and due to that the increase in the track width results in a visible decrease in the height of the clad layer. The results are almost identical on the low and high speed. This opens the possibility of controlling the geometric parameters of the track through the contact angle and the substrate parameters that influence on it independently on the scanning speed.

Figure 3 shows the distribution of the average size of the crystallites in the track cross sections for two values of the contact angle. Just as in the case of a cladded drop, the average crystallite size is larger with increasing contact angle. This is due to the fact that the melt pool is more developed in the case of a low contact angle. A small increase in the track width above the laser beam width leads to the activation of transverse currents. An increase in the contact angle constrains the fluid flow in the melt pool. The current does not have time to develop so the cooling rates are somewhat lower.
4. Conclusion
The developed model allows estimating the clad layer microstructure taking into account the experimentally measured contact angle of the track and the substrate. The parameters of the substrate that influence the contact angle could be taken into account in such model. The spreading behavior of cladded tracks is shown for various processing conditions. The powder jet radius showed dissimilar response to the contact angle change depending on the comparison to the melt pool width. In the case of wide powder jet the increase of the contact angle decreases the track width and the catchment efficiency but the height is remained constant. The decrease of track width is accompanied with height increase in the case of narrow powder jet. The possibility of LC of tracks with the same geometric parameters and at the same time a different microstructure is determined. It is shown that an increase in the contact angle of the melt leads to an increase in the average size of the crystallites in the deposited layer. Results can be used for the process planning and optimization of LC.

5. References
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Acknowledgments
This work was supported by the Federal Agency of Science Organizations (agreement № 007-GZ/Ch3363/26)