Multiscale Modelling of Laser Beam Welding.

Part I: Macroscopic and Mesoscopic Scale

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The process of the laser beam welding of Al-Mg-Si alloy is simulated on the different length scales. The first part of the work considers the reconstruction of the heat input distribution and the weld pool shape on the macroscopic scale as well as the simulation of the grain structure on the mesoscopic scale. The reconstruction of the heat input distribution and the weld pool shape is realised using the technique of the inverse modelling. The grain structure is simulated using the method of the grain boundaries evolution. The results of the simulation are found to be in a good agreement with the experimentally observed macroscopic and mesoscopic features of the laser beam welds. It is shown that using the coupled macroscopic-mesoscopic algorithm of calculation can sufficiently improve the accuracy of the inverse modelling.

1 Introduction

The technological properties of laser beam welds are formed due to the simultaneous effects of different physical phenomena which occur on different length scales:

(i) macroscopic (the order of magnitude of 0.1-1 mm): temperature distribution, temperature gradient, cooling rate, stresses, distortion, etc.;
(ii) mesoscopic (the order of magnitude of 10-100 \( \mu \)m): grain size, texture, etc;
(iii) microscopic (the order of magnitude of 1-10 \( \mu \)m): primary and secondary dendrite arm spacing, morphology, microsegregation.

Correspondingly, the simulation of technological properties of laser beam welds requires the multiscale approach. This means that the transfer of the correspondent boundary conditions between the codes simulating the physical processes on different scales should be realised. The present paper describes a multiscale approach for the simulation of the laser beam welding on macro- and mesoscopic scale.

2 Direct and Inverse heat conduction problem

The heat source (laser beam) with volumetric power density \( q_{3 \text{ net}} \) is assumed to move uniformly and linearly with constant velocity \( v \). The equation for the conservation of
energy with consideration for the latent heat and the convection in the weld pool can be written as

\[
c_p \frac{\partial T}{\partial t} = \text{div}(\lambda \text{grad} T) - c \rho \left[ \left( w_x - v \right) \frac{\partial T}{\partial x} + w_y \frac{\partial T}{\partial y} + w_z \frac{\partial T}{\partial z} \right] + q_{3L} + q_{3\text{net}} \quad (1)
\]

where \( c \) is the specific heat capacity, \( \rho \) is the density, \( \lambda \) is the thermal conductivity, \( w_x, w_y \) and \( w_z \) are the components of the convective velocity of the fluid, \( q_{3L} \) is the latent heat per unit volume. The first three terms on the right-hand side of the equation (1) account for heat conductivity, convection and latent heats of fusion and solidification, respectively.

If the temperature field does not change in a moving reference frame (steady state, \( \partial T/\partial t = 0 \)) then equation (1) can be presented as

\[
div(\lambda \text{grad} T) + c \rho v \frac{\partial T}{\partial x} + q_{3\text{app}} = 0 \quad (2)
\]

where

\[
q_{3\text{app}} = q_{3\text{net}} - c \rho \left[ w_x \frac{\partial T}{\partial x} + w_y \frac{\partial T}{\partial y} + w_z \frac{\partial T}{\partial z} \right] + q_{3L} = q_{3\text{net}} + q_{3c} + q_{3L} \quad (3)
\]

The apparent source \( q_{3\text{app}} \) represents the simultaneous influence of the real source \( q_{3\text{net}} \) as well as convection \( q_{3c} \) and latent heat \( q_{3L} \). Equation (2) is analogous to the well-known quasi-stationary equation for solids if \( q_{3\text{app}} \) is considered to mean some apparent (equivalent) volumetric heat source. Equations (2) and (3) with the corresponding boundary conditions present the formulation of a direct heat conduction problem.

The reconstruction of the welding conditions on the basis of the experimentally observed or desired properties of the weld relates to the inverse problem [1-3]. For example, the solution of the inverse heat conduction problem (IHCP) allows to reconstruct the heat distribution \( q_{3\text{app}}(x,y,z) \) and other welding conditions.

The following augmented sum-of-squares function (objective function) is taken to be a criterion of IHCP solution accuracy:

\[
F(p) = \sum_{j=1}^{J} w_f^j \left( f_j^m - f_j(p) \right)^2 + \sum_{k=1}^{K} w_p^k \left( p_k - p_k^0 \right)^2 + w_q \left( q_{\text{net}}^m - q_{\text{net}}(p) \right)^2 + R.T. \quad (4)
\]

where \( J \) is the total number of observations, \( K \) is the total number of unknown parameters, \( p_1, p_2, \ldots, p_K \) are the unknown parameters, \( f_j^m \) and \( f_j \) are the measured and calculated values of the response functions, \( w_f^j, w_p^k \) and \( w_q \) are the weighting factors, \( q_{\text{net}}^m \) and \( q_{\text{net}} \) are the measured and calculated net power, \( R.T. \) is the regularisation term [2].
The unknown parameters $p_1$, $p_2$, ..., $p_K$ are estimated utilising the method of least squares, i.e. minimising the objective function $F$ with respect to each parameter. The corresponding set of nonlinear equations is solved in the iterative fashion, based on the use of sensitivity coefficient algorithm [2-3].

3 Heat input reconstruction (macroscopic scale)

The heat input reconstruction was carried out for the welds produced on the edge of the 1.15mm AC 120 aluminium alloy sheets (Fig. 1). The edge melting imitates fairly well the edge welding as well as the butt laser welding of thin plates.

The peak temperature $T_{\text{max}}$ under weld depth $H$ and the texture orientation angle $\gamma$ are taken as the measured values of response function $f^{m}$ (Fig. 1b). The depth $H$ has been determined using the standard metallography. Experimental examination of the texture orientation has been carried out with an accuracy of 2.5° using X-ray diffraction analysis. The evaluation of the texture orientation angle $\gamma$ requires a special simulation technique on the mesoscopic scale (see below). For these calculations, the temperature gradient angle $\beta$ (see Fig. 1b) was assumed to represent the calculated texture orientation.
Figure 1. Laser edge melting: (a) piecewise-linear continuous distribution of apparent power density along the sheet edge and (b) the parameters related to the formulation of the inverse heat conduction problem.

For simplification, the apparent volumetric source was reduced to the apparent area source $q_{2\text{ app}}(x)$ acting on the plate edge (Fig. 1a). The last assumption is appropriate, since the weld pool is relatively long, i.e. the length greatly exceeds the width. The source $q_{2\text{ app}}(x)$ is represented as a piecewise-linear continuous function. The unknown parameters are the values of $q_{2\text{ app}} n$ at points with coordinates $x_n (n = 1,...,N; K=N)$.

Figure 2 shows an example of the reconstructed weld pool shape together with the correspondent distribution of apparent power $q_{2\text{app}}(x)$. The heat distribution has an expected maximum at the front part of the pool which corresponds to the thermal effect of the laser beam. The rise of the apparent power at the end of the weld pool clearly exhibits the maximal release of the latent heat of solidification in this region.
Figure 2. Results of the solution of the inverse heat conduction problem: (a) apparent power density distribution and (b) weld pool shape (thickness $H = 1.15$ mm, velocity $v = 50$ mms$^{-1}$, laser beam power $q_{\text{gross}} = 1700$ W).

The values of the temperature gradients and cooling rates calculated on the basis of the reconstructed temperature fields were of the order of magnitude of 50-400 K/mm $1000$ K/s -12000 K/s respectively. These parameters have been used as the macroscopic background conditions for the microscopic simulation (see the second part of the present paper).

4 Simulation of the grain structure (mesoscopic scale)

For the reconstructed temperature distribution the grain structure of the laser beam welds can be simulated using the grain boundary evolution method [4]. The examples of the simulated grain structures are represented in Fig. 3 together with the photographs of the grain structure observed in experiments.

5 Coupled macro-mesoscopic simulation

Good qualitative agreement between the calculated grain structures and the observed ones does not mean the excellent accuracy of the weld pool reconstruction. It can be clearly seen by comparison of the segregation lines on the experimental photograph with the reconstructed shape of the weld pool (Fig. 3a). It is clearly seen that the reconstructed weld pool is longer as it was in reality. The relatively low accuracy usually relates to the simplification introduced in the formulation of the inverse problem. In this case it was the assumed estimation of the texture orientation angle $\gamma$ using the temperature gradient angle $\beta$, which is close to the angle $\gamma$, but does not coincide with it. Utilising the coupled macro-mesoscopic simulation described below allows overcoming such simplifications and sufficiently increasing the accuracy of the weld pool reconstruction.
Figure 3. Results of the mesoscopic simulation: simulated and observed grain structures (longitudinal sections) under different welding speeds.

The distribution of the texture orientation angle $\gamma$ can be derived from the grain structure calculated on the mesoscopic scale [5]. The calculated value $\gamma(y)$ represents the mathematical expectation of $\gamma$-distribution at a certain distance $y$ from the plate edge (Fig. 4). It is seen that this angle is higher than the temperature gradient angle. The difference between the angles $\gamma$ and $\beta$ is likely caused by the mechanism of the grain selection [5].
If the calculated value $\gamma(y)$ is taken in the formulation of the inverse problem instead of the temperature gradient angle $\beta$, the accuracy of the weld pool reconstruction is much higher (compare Fig. 5a and Fig. 5b). In this case, the coupled macro-mesoscopic simulation is realised. That is, each iteration step of solving the inverse problem includes a solution of two direct problems on different scales: the heat transfer problem on the macroscopic scale and the evaluation of the texture orientation derived from the simulated grain structure on the mesoscopic scale.

**Figure 4.** Distribution of the temperature gradient angle $\beta$ and the texture orientation $\gamma$. If the calculated value $\gamma(y)$ is taken in the formulation of the inverse problem instead of the temperature gradient angle $\beta$, the accuracy of the weld pool reconstruction is much higher (compare Fig. 5a and Fig. 5b). In this case, the coupled macro-mesoscopic simulation is realised. That is, each iteration step of solving the inverse problem includes a solution of two direct problems on different scales: the heat transfer problem on the macroscopic scale and the evaluation of the texture orientation derived from the simulated grain structure on the mesoscopic scale.
Figure 5. Influence of the coupled macro-mesoscopic simulation on the accuracy of the weld pool and grain structure reconstruction: (a) uncoupled simulation and (b) coupled simulation.

6 Conclusions and future developments

The inverse modelling based on the multiscale approach seems to be a promising tool for investigation and optimisation of properties of the laser beam welds. On the basis of a relatively simple case of the edge welding, the present approach has shown the possibility to reconstruct the process conditions (heat input distribution, weld pool shape) as well as the correspondent grain structure. It is also shown, that the higher accuracy is provided by utilisation of the coupled multiscale simulations. The developed approach can be used for the evaluation of the heat input efficiency, and, what is more promising, for the optimisation of the welding conditions in accordance with some prescribed (desired) properties (for example, the desired grain structure or the microstructure).

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Appendix

Table: Properties of the AC 120 aluminium alloy used for simulation.
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<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Thermal conductivity $\lambda$, W m$^{-1}$ K$^{-1}$</td>
<td>175</td>
</tr>
<tr>
<td>Density $\rho$, kg m$^{-3}$</td>
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</tr>
<tr>
<td>Specific heat capacity $c$, J kg$^{-1}$ K$^{-1}$</td>
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</tr>
<tr>
<td>Solidus temperature $T_S$, K</td>
<td>858</td>
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<tr>
<td>Liquidus temperature $T_L$, K</td>
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<tr>
<td>Heat transfer coefficient $\alpha$, Wm$^{-2}$K$^{-1}$</td>
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</tr>
<tr>
<td>Plate thickness $h$, mm</td>
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<td>Laser beam power $q_{\text{gross}}$, W</td>
<td>1700</td>
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<tr>
<td>Welding speed $v$, mm s$^{-1}$</td>
<td>16.7, 25, 50</td>
</tr>
</tbody>
</table>

References


