Simulation Of Phase Transformations In Steel Parts Produced By Laser Powder Deposition

L. Costa, R. Vilar, T. Reti, R. Colaço, A. M. Deus, I. Felde
Simulation Of Phase Transformations In Steel Parts Produced By Laser Powder Deposition

L. Costa¹, R. Vilar¹, T. Reti², R. Colaço¹, A. M. Deus¹, I. Felde³

¹ DEMat, Instituto Superior Técnico, Av. Rovisco Pais, 1049-001 Lisboa, Portugal
² Szchenyi Istvan University, Egyetem ter 1., H-9026 Györ, Hungary
³ Bay Zoltán Institute for Materials Science and Technology, Fehérvári u. 130, H-1116 Budapest, Hungary

Keywords: rapid manufacturing, laser powder deposition, tool steels, phase transformations, hardness, finite element analysis.

Abstract. Multilayer laser powder deposition is being used for the rapid manufacturing of fully dense near net shape components in a wide variety of materials. In this process parts are built by overlapping consecutive layers of a laser melted material. As a result of this overlapping, the material in each layer will undergo successive thermal cycles as new layers are deposited. Despite their short duration, these thermal cycles can activate solid-state transformations that lead to progressive modification of the microstructure and properties of the material. Since the thermal history of the material in the deposited part will differ from point to point, the part will present a complex and heterogeneous microstructure, and properties that differ from point to point. Given that the microstructure and property distribution in steel parts produced by laser powder deposition can only be predicted by modelling, a three-dimensional thermo-kinetic finite element model of laser powder deposition of tool steels was developed. In the present work this model was applied to the study of the influence of substrate size on the microstructure and properties of a six-layer wall of AISI 420 tool steel. The results show that the temperature field depends significantly on the size of the substrate, leading to distinct microstructures and properties in the final part.

Introduction

Laser powder deposition (LPD) [1-4] is a very promising technique for the rapid manufacture of fully dense steel components. Although the advantages of this flexible manufacturing process are widely recognised [1-5], there are still some factors restraining its wide acceptance by industry. Controlling and tailoring the material properties of the final part is one such factor. These properties are significantly affected by the solid-state transformations that may occur during deposition, induced by the consecutive thermal cycles created by successive layer overlapping. The lack of detailed understanding of these transformations and of their influence on the final properties of the deposited part may lead to irreproducible results. In order to ensure that the final part possesses an appropriate microstructure, one must know the effect of the processing parameters and part build-up strategy on the thermal cycle and microstructural changes. This knowledge cannot be obtained by trial and error, due to the large number of processing parameters that must be considered. Also, the results of such an approach might not be directly applicable to all cases because the specific geometry of individual parts strongly affects the thermal field in the part and its time evolution. A more satisfactory approach relies on computer aided engineering techniques, such as finite element analysis [6-9]. This approach requires a model describing the time evolution of the thermal field in the part during the deposition process, as well as a detailed knowledge of the solid-state phase transformations that occur in laser processed steels. The latter information is available in the work of several authors [10-15] on laser processed tool steels. In particular, Colaço et. al [11] showed that, due to their fast solidification and cooling rates, laser processed tool steels may contain
significant proportions of metastable phases, in particular austenite and martensite, that will evolve when the material is reheated [12].

In the present work, a model to simulate multilayer LPD of tool steels is described. The model couples heat transfer finite element calculations carried out using the ABAQUS software package [16] with phase transformation kinetics data on the martensitic transformation, tempering and austenitization to simulate the phase transformations that occur in the material during deposition and the resulting changes in hardness. Using this model, the effect of the size of the substrate on the evolution of the temperature field, microstructure and properties of the processed material during the deposition of a six-layer wall of AISI 420 tool steel (0.33 %C, 13.5 %Cr) was studied.

Figure 1. During laser powder deposition a material in powder form is injected into the path of a laser beam and melted simultaneously with a thin layer of the substrate to form a continuous track of material. The partial overlapping of individual tracks in a suitable pattern produces a continuous layer of material. By overlapping such layers, three-dimensional objects are generated.

**Heat Transfer Analysis**

In the heat transfer calculations it was assumed that the base material is initially at room temperature, $T_0$. On the other hand, theoretical results of Neto and Vilar [17] show that the energy absorbed by the powder particles as they fly across the laser beam can be sufficient for them to reach the liquidus temperature before entering the melt pool. Therefore, in the present work it was assumed that the finite elements which are activated at the beginning of each deposition step (Fig. 2) are at the liquidus temperature of the steel. The boundary conditions take into consideration heat losses due to surface convection and radiation. Heating of the surface by a focused Gaussian laser beam (TEM$_{00}$ mode) was simulated by applying a surface heat flux (described by Eq. 1), which depends on the laser beam power, $P$, laser beam radius, $r_L$, and radiation absorption coefficient of the material, $\alpha$.

$$F_{\text{Laser}} = \alpha \cdot F_0 e^{-\frac{2\pi^2 r^2_L}{P}}, \quad F_0 = \frac{2 \cdot P}{\pi \cdot r^2_L}. \quad (1)$$

Figure 2. The finite element analysis of laser powder deposition was performed sequentially as a series of constant geometry problems (called steps), linked together by introducing the output of problem $n$ as initial conditions for problem $n+1$. At the beginning of each step a new group of finite elements is activated and the boundary conditions are updated according to the newly exposed surfaces (represented by the thick black lines).

**Modelling of phase transformations**

The model assumes that melting, solidification, transformation of austenite into martensite, martensite tempering and partial or total austenitization may all occur during LPD of tool steels, depending on the local thermal cycle. The kinetics of these phase transformations was described using semi-empirical models presented below.
Martensitic transformation. Solidification of laser processed AISI 420 tool steel leads to the formation of austenite and solidification occurs with a dendritic solid-liquid interface [11]. As a result, after solidification, the microstructure consists entirely of austenite dendrites. This phase was considered to be chemically homogeneous. Due to the high cooling rate observed in LPD, diffusive solid-state transformations are usually suppressed during cooling to room temperature. As a result, the austenite resulting from solidification can only transform into martensite. The martensitic transformation starts as soon as the temperature drops below the martensite start temperature, Ms, and the volume fraction of martensite increases with undercooling. The volume fraction of martensite, \( f_M \), was calculated using the Koistinen and Marburger [18] equation (Eq. 2), where \( f_{\gamma 0} \) is the initial volume fraction of austenite. The Ms temperature was calculated from the chemical composition of the steel, using Andrews’ [19] equation (Eq. 3). The chemical element designations in Eq. 3 refer to concentrations in wt. %. For steel with 0.33 %C and 13.5 %Cr, the Ms temperature is 160 °C.

\[
f_M = 1 - f_{\gamma 0} \cdot \Phi(T), \quad \Phi(T) = \begin{cases} 1 & \text{if } T \geq Ms \\ \exp\left(-0.011 \cdot (Ms - T)\right) & \text{if } T < Ms \end{cases}
\]  

(2)

\[
Ms_{ANDREWS} = 512 - 453 \times (%C) - 15 \times (%Cr).
\]  

(3)

Diffusive transformations: tempering and austenitization. After cooling to room temperature, the newly deposited material presents a microstructure consisting of martensite and austenite. Reheating leads to tempering of the martensite. Martensite will decompose into ferrite and cementite (\( M \rightarrow \alpha + \text{Fe}_3\text{C} \)) in the temperature range of 200 to 350 °C. As the temperature rises above 500 °C, precipitation reactions leading to the formation of \( M_7\text{C}_3 \) and \( M_{23}\text{C}_6 \) carbides will be activated [20]. Simultaneously, \( \text{Fe}_3\text{C} \) particles will dissolve in the matrix. If the temperature exceeds Ac1, ferrite will transform into austenite, which will progressively dissolve the carbides. The volume fraction of austenite increases with temperature to reach 100% at Ac3 temperature. In the model it was assumed that this variation is linear. As before, austenite is considered chemically homogeneous. Since the heating rates characterizing the LPD process are extremely high, Ac1 and Ac3 temperatures will present hysteresis, shifting away from their equilibrium values. To take hysteresis into account, the Ac1 and Ac3 temperatures of AISI 420 steel were considered to be 875 °C and 1015 °C respectively, based on experimental data of Rose et al [21]. The microstructure of a multilayer part at room temperature will then present different proportions of martensite, austenite, ferrite and carbides, depending on the thermal cycles observed in the part. It was assumed that a martensitic transformation will only occur if new austenite is formed during reheating, i.e. if the temperature rises above Ac1, thus neglecting destabilization of retained austenite during tempering and its transformation into martensite upon subsequent cooling [12].

The average hardness of the material was considered to be the weighted average of the hardness of individual phases (Eq. 4), where \( f_\gamma \) is the volume fraction of austenite and \( H_\gamma \) and \( H_{(M \rightarrow \alpha + \text{carbides})} \) are the hardness of austenite (280 HV) and tempered martensite, respectively. Reti et al [22] showed that softening of steel due to anisothermal tempering can be estimated using Eq. 5, where \( H_0 \) is the hardness of martensite, \( R \) the universal gas constant and \( A \) and \( m \) fitting constants. Since several competitive reactions may occur simultaneously, the activation energy, \( Q \), was replaced by an effective activation energy (Table 1), as suggested by Mittemeijer [23]. For AISI 420 steel the values of these parameters were estimated on the basis of data collected from isothermal tempering experiments performed by the authors, leading to the values for the effective activation energy presented in Table 1 and to \( H_0 = 658 \) HV, \( A = 1300 \) HV/s and \( m = 0.055 \).

\[
H = f_\gamma \cdot H_\gamma + (1 - f_\gamma) \cdot H_{(M \rightarrow \alpha + \text{carbides})}.
\]  

(4)
\[ H_{(M \rightarrow \alpha+\text{carbides})} = H_0 - A \cdot \left[ \int_0^\infty e^{-Q/R_T(t)} \cdot dt \right]^{\alpha}. \]

(5)

### Table 1. Values of effective activation energy, Q, for tempered AISI 420 tool steel.

<table>
<thead>
<tr>
<th>T [ºC]</th>
<th>20</th>
<th>300</th>
<th>400</th>
<th>500</th>
<th>600</th>
<th>700</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q [kJ/mol]</td>
<td>220</td>
<td>220</td>
<td>250</td>
<td>320</td>
<td>250</td>
<td>250</td>
</tr>
</tbody>
</table>

**Case study - effect of part size on the final properties of the material**

The model described in the previous section was used to study the influence of the substrate size on the final microstructure and properties of a six-layer 1 mm thick wall of AISI 420 tool steel, deposited by LPD (Fig. 3). The deposition parameters were: scanning speed = 20 mm/s, powder feed rate = 0.1 g/s and powder use efficiency = 78%. For a track width of 1.0 mm, these processing conditions allow two cubic elements of 0.5³ mm³ to be activated every 25 ms. A total of six overlapping single tracks were deposited on a substrate of the same steel (Fig. 3). Each track has a length of 10.0 mm, a thickness of 0.5 mm and a width of 1.0 mm. The idle time between consecutive layers was 2 seconds. It was assumed that the base material is in the pre-treated condition (quenched and double tempered for 1h at 200 ºC), with an initial microstructure of ferrite and carbides and a hardness of 560 HV. The initial temperature of the deposited material was 1450 ºC, while the substrate was initially at 20 ºC. The Gaussian laser beam was focused into a spot with 3 mm diameter, measured at e⁻² of maximum intensity. An effective laser beam power \(P' = \alpha \cdot P = 325\) W was used, where \(\alpha\) is the average absorptivity. Average values of thermal conductivity and specific heat calculated from the properties of individual phases (Table 2), weighed by their volume fractions in the microstructure, were used for each element.

![Figure 3. Finite element mesh used to simulate the multilayer LPD of a 6 layer wall. The analysis was performed for L=30.5 mm and L=4.0 mm. The smallest finite elements are located in the regions where thermal gradients are expected to be high. A symmetry plane exists if the wall is built up along the mid-plane of the base material. In this case, only ½ of the global problem has to be solved if a zero heat flux boundary condition is imposed along the symmetry plane.](image)

**Results and discussion**

The results obtained are presented in figures 4 to 6. The data provided concerns the symmetry plane of the wall (Fig. 3). The results confirm that the processing parameters used in the calculations are realistic, producing an adequately sized melt pool, with limited melting of the previous layer (Fig. 4a and b). The temperature distribution is strongly influenced by the size of the substrate, which affects its ability to extract heat from recently deposited material. In the part deposited on the smaller substrate, heat builds up during deposition and the temperature in each layer of the wall does not drop below the martensite start temperature prior to the deposition of the next layer. As a result the martensitic transformation will only occur after completion of the deposition process, when the whole part cools to room temperature. In this case, the deposited material consists mostly of martensite and some retained austenite and presents a hardness distribution that is reasonably uniform over the part (Fig. 6a). Tempering is only observed in the first layers, deposited before heat...
could build up in the part. In the case of a large substrate, heat does not accumulate to the same extent and each deposited layer cools down below the Ms temperature (and partially transforms into martensite) before the addition of a new layer (Fig. 5b). As further layers of material are added, the martensite in previous layers evolves by cumulative anisothermic tempering and its hardness is correspondingly reduced (Fig. 6b). As a result, the final material presents a non-uniform hardness distribution over the part height. The maximum hardness is found in the upper layers, which consist of untempered martensite and austenite. Conversely, martensite in the first layers has been extensively tempered and its hardness is lower.

Conclusions
A simple three-dimensional thermo-kinetic finite element model of multilayer laser powder deposition has been developed and implemented. The deposition of a six layer wall of AISI 420 tool steel on differently sized substrates was analysed. The temperature field, volume fraction of the phases formed and average hardness of the material were calculated. The simulation results show that two identical parts, deposited using the same processing parameters and building-up strategy, can present different microstructures and properties. The difference in the final outcome is due to the influence of the substrate size on its heat extracting capability, which affects the time evolution of the temperature field during deposition. A small substrate leads to a material microstructure consisting mainly of untempered martensite and retained austenite and presenting a reasonably uniform hardness over the part height. A larger substrate leads to a more heterogeneous microstructure consisting of fresh martensite, tempered martensite, austenite, ferrite and carbides.

Appendix
Table 2 - Material properties used in the finite element analysis [24, 25].

<table>
<thead>
<tr>
<th>Temperature [ºC]</th>
<th>27</th>
<th>300</th>
<th>600</th>
<th>800</th>
<th>900</th>
<th>1100</th>
<th>1300</th>
<th>1410</th>
<th>1425</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal conductivity [W/m·K]</td>
<td>M, α</td>
<td>43.1</td>
<td>36.7</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>γ</td>
<td>15.0</td>
<td>18.0</td>
<td>21.7</td>
<td>25.1</td>
<td>26.8</td>
<td>28.9</td>
<td>32.8</td>
<td>34.0</td>
</tr>
<tr>
<td>Specific heat [J/kg·K]</td>
<td>M, α</td>
<td>485</td>
<td>574</td>
<td>654</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>γ</td>
<td>535</td>
<td>568</td>
<td>603</td>
<td>632</td>
<td>-</td>
<td>760</td>
<td>750</td>
<td>-</td>
</tr>
<tr>
<td>Density [kg/m³]</td>
<td>-</td>
<td>7750</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Latent heat of fusion [kJ/kg]</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>250</td>
</tr>
</tbody>
</table>

M – martensite; α - ferrite; γ - austenite

Acknowledgements

The authors are grateful to GRICES and OMFB for financial support (project: Repairing of machine parts by laser cladding – Proj. 4.1.1). The author, Lino Costa, thanks Fundação para a Ciência e Tecnologia for financial support.

References