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On the importance of heat source modeling for controlling molten pool geometry during laser surface treatment of Ti6Al4V alloy

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Abstract. Laser surface treatment is a precise method for modifying the microstructure and surface properties of materials, including Ti-6Al-4V, by adjusting laser parameters to enhance characteristics such as wear and fatigue resistance. However, the complexity of laser-material interactions, particularly the thermal effects, introduces challenges in predicting the thermal distribution and resulting material properties. This study compares two heat source models - the conventional 3D conical Gaussian heat source model and the more recent elliptic paraboloid volumetric heat source model - for their ability to accurately simulate laser surface treatments. The models were validated by comparing numerical simulations with experimental data on thermal field and on molten pool width and penetration depth obtained from metallographic analysis. The results show that both models yield stable predictions, with the elliptic paraboloid model providing more accurate representations of the laser track profile. This model, which better adapts to elliptical heat distributions, is particularly beneficial for micro and nanoscale surface functionalization, where small discrepancies in thermal treatment can significantly affect material behavior. Additionally, a different methodology for modeling the heat source based on process temperature, rather than traditional geometric heat flux definitions, was proposed.

Introduction

Among various surface modification methods, laser treatment is notable for its high precision to induce localized changes in microstructure and surface geometry, in fact by controlling laser parameters it is possible to modify surface morphology and its mechanical properties effectively. In the case of Ti-6Al-4V, laser surface treatments can enhance surface characteristics like wear and fatigue resistance preserving the material's structural integrity [1-5]. Several researches has been dedicated to study the metallurgical influence of laser texturing on surface properties of Ti-6Al-4V, with numerous studies on corrosion resistance and surface durability [6-8]. However, the complexity of laser-material interactions, especially the thermal effects, presents notable challenges. The rapid cycles of heating and cooling trigger complex thermo-mechanical responses within the material, resulting in residual stresses that can affect bulk properties such as toughness and fatigue resistance [9-11]. For this reason, developing numerical models capable of accurately predicting the thermal-affected zone of the workpiece is essential, as they provide critical insights into its geometry, mechanical properties, and temperature distribution. Detailed simulations allow for the estimation of key factors such as laser penetration depth, heat-affected zone (HAZ) formation and oxide distribution, ultimately reducing the need for costly and time-consuming experimental trials [12-14]. Nascimento et al. [15] highlighted the importance of mathematical modeling of the heat source in joining processes for performing accurate simulations and

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predicting the final mechanical characteristics, thermal stresses and potential failure risks. Mackwood and Crafer [16] published a comprehensive review on the thermal importance of modeling of welding heat sources. Chukkan et al. [17] demonstrated that conventional heat source models can yield less accurate results when simulating the molten pool shape during laser welding of 316L stainless steel. Li et al. [18] developed a hybrid heat source model that significantly improved the accuracy of numerical simulations for selective laser melting (SLM) of IN625. These studies emphasize the critical role of selecting an appropriate computational model to gain a thorough understanding of the fundamental phenomena driving the process. This research aims to expand on this body of knowledge by conducting a comparative numerical and experimental analysis to identify the most suitable heat source model for accurate surface functionalization. The analysis will compare a conventional heat source model with a recently proposed alternative, since conventional heat source models, typically relying on bulk heating or simple radiant heat sources, have limitations in achieving the precision and uniformity required for modern biomedical materials. These conventional methods can result in uneven heating and difficulties in achieving the desired functionalization since do not well fit the obtained experimental laser track. Furthermore, the study introduces an innovative methodology for modeling the heat source based on process temperature, as opposed to the traditional approach of defining the geometric location of the heat flux. Also, the specific model proposed herein, is used for industrial application with the aim to be adapted for the surface functionalization of injection moulding devices reducing problems of energetic loss and product defects.

Experimental method

Laser irradiation was conducted on Ti6Al4V (Table 1) by an air-cooled ytterbium fiber laser system with a maximum average power of 100 W and a wavelength of 1064 nm. The laser beam was focused onto the surface via an F-theta lens (f = 160 mm), producing a focused spot with a diameter of 55 μm. The following processing parameters were maintained constant throughout the experiments: a pulse frequency (f) of 1 MHz, an average power (P) of 80 W and a laser scanning speed (v) of 30 mm/sec.

Table 1 – Ti6Al4V chemical composition (weight %).

Elements	Ti	Al	V	O	Fe	N	C	H	Y	Each	Total
Weight %	Bal	6.31	4.25	0.17	0.13	0.021	0.014	0.001	<0.001	0.10	<0.4

To ensure result reliability the experiment was replicated three times. Thermal data during the process was captured using a FLIR A655sc Infrared Camera (IRC), with a temperature range of 100 to 650 °C to focus on the thermal cooling phase, which has a longer duration. The material's emissivity was calibrated by comparing infrared camera measurements with those from a thermocouple on a sample heated in controlled temperature steps, yielding an emissivity value of 0.36. Temperature data were taken along the entire treated line, and an iterative trial-and-error method was used to calibrate the temperature and convection coefficient in the SFTC DEFORM-3D^{TM} software, which modeled the laser heat source. After treatment, three samples were cut from each test, resulting in a total of 9 samples. These were analyzed via optical microscopy, focusing on the molten pool width and laser penetration depth. Fig. 1 presents a micrograph from optical microscopy, along with the geometric parameters used to characterize the laser process cross-section: molten pool width and depth.

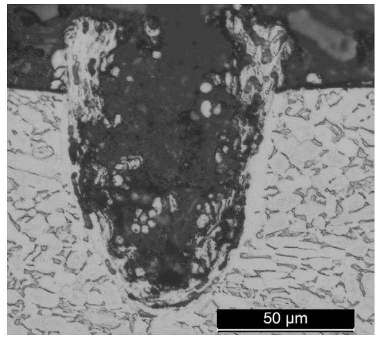

Figure 1 – Optical microscopy image of the transverse section of the laser-treated surface.

Numerical modeling

The commercial FE software SFTC DEFORM-3D^{TM} (Fig. 2) was employed to simulate the laser processing, with the workpiece modeled as a plastic body consisting of 360,000 tetrahedral elements.

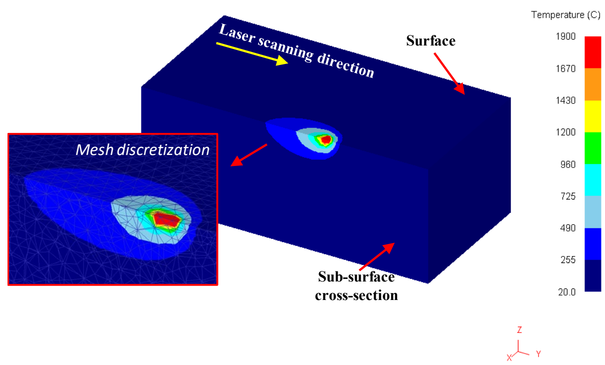

Figure 2 – Finite element modeling showing the heat source movement across the surface and subsurface by a workpiece sliding view (section along x axis).

Two distinct heat source models were used to represent the laser surface treatment: a conventional 3D conical Gaussian heat source model [19], initially proposed in 1996, and an elliptic paraboloid volumetric heat source model introduced by García-Gracía in 2016 [20], which offers enhanced adaptability for elliptical heat shapes.

In the case of the 3D conical Gaussian heat source model, the parameters r_e and r_i represent the upper and lower radii, respectively, while z_e and z_i denote the cone's height (Fig. 3a). For the elliptic paraboloid volumetric heat source model, r_0 refers to the radius of the circular base of the paraboloid, and c is the length of the paraboloid in the direction of the laser penetration (Fig. 3b).

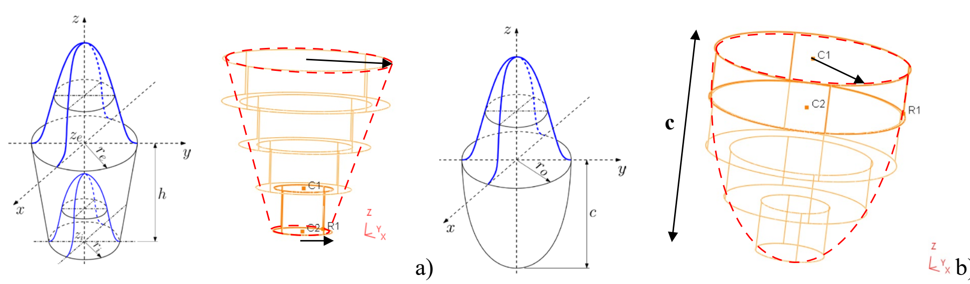

Figure 3 – Measurements of heat source model parameters for a) 3D Gaussian conical volumetric and b) elliptic paraboloid volumetric shape.

Both heat source models were implemented using a series of 3D heat exchange windows that replicated the specified heat distribution, corresponding to an experimental movement velocity of

30 mm/s. All heat source parameters were determined by analyzing the experimental micrographs, while the temperature and convection coefficients of the heat exchange windows were calibrated using a trial-and-error procedure, comparing the results with experimental data on molten pool width, penetration depth and temperature profiles.

FE validation and results

The FE model was validated by comparing the simulation results with experimental data. As shown in Fig. 4, both heat source models yield stable numerical results, producing consistent simulated thermal fields that result in a characteristic comet-tail profile.

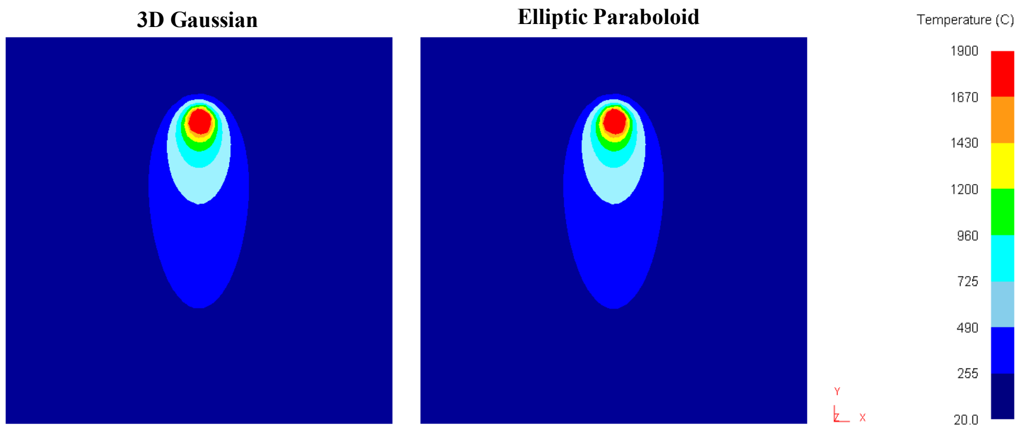

Figure 4 – FE temperature distribution.

Fig. 5 presents a comparison between the simulated molten pool width and penetration depth, alongside the corresponding experimental results obtained from metallographic analysis, confirming the accuracy and reliability of the proposed heat source models.

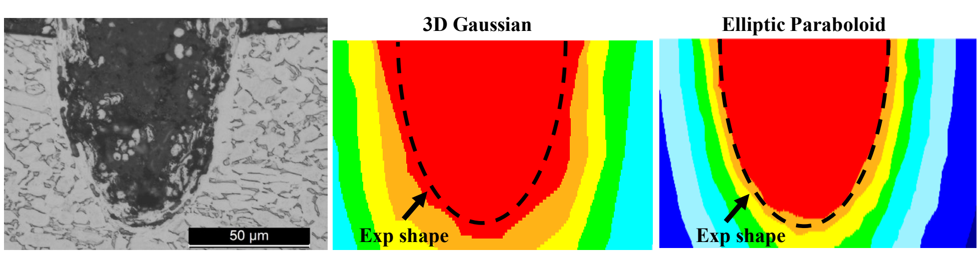

Figure 5 – FE molten pool validation.

A detailed analysis is provided in Fig. 6, where the experimental measurements of the molten pool dimensions are compared with the numerical values obtained from both the adopted models.

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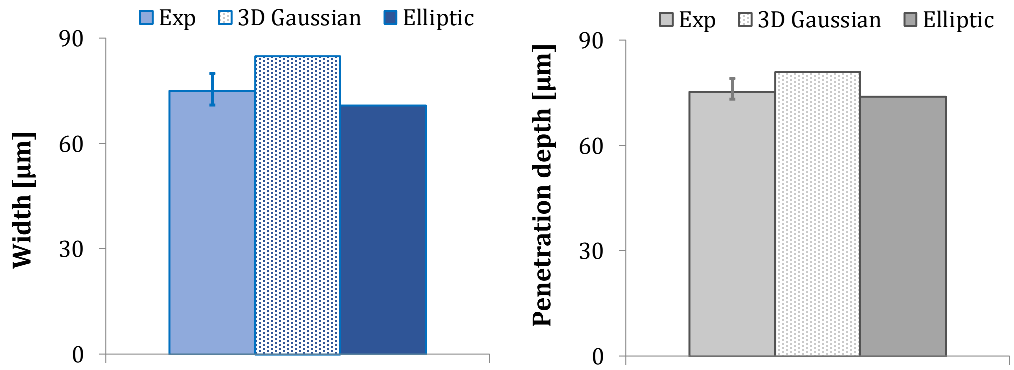

Figure 6 – FE laser track geometry validation.

The slight discrepancies observed between the numerical and experimental results for both investigated models can be attributed to: (i) the iterative calibration process for defining heat source constants, (ii) the heat source distribution, and (iii) the material discretization. Specifically, a relative error of 13% and 8% was observed for the width and penetration depth, respectively, when using the 3D conical Gaussian heat source model. While, a relative error of 6% and 2% was also observed for the width and penetration depth when using the elliptic paraboloid model. It is evident that the elliptic paraboloid volumetric heat source model exhibits a smaller error.

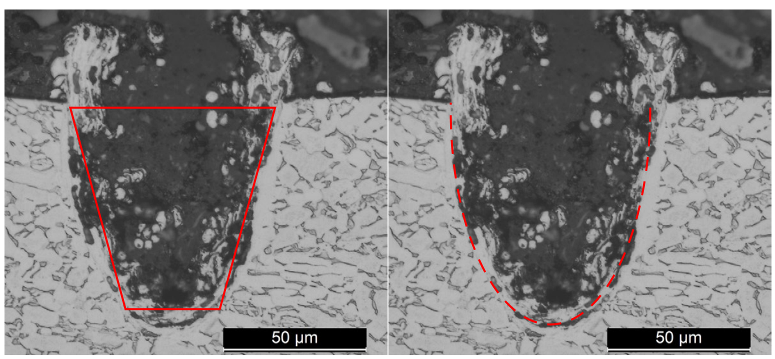

Figure 7 – FE molten pool geometry fit for a) 3D Gaussian conical and b) elliptic paraboloid volumetric shape.

As shown in Fig. 7, its mathematical formulation allows for a more accurate representation of the track line profile. In fact, it is evident that the numerical curve of the 3D Gaussian formulation is narrower than the actual profile. This is why, during the calibration phase, the optimal compromise between shape fitting, penetration depth and molten width led to the aforementioned errors, which correspond to the calibration with the lowest error margin. This aspect is particularly significant, especially when surface functionalization is performed at the micro/nanoscale, where even small discrepancies between the numerical and experimental thermal treatments can play a crucial role in achieving the desired surface functionalization. The results clearly demonstrate that the adoption of a modern heat source model provides more precise and uniform control over the temperature at specific points on the material surface, minimizing the impact of heat on surrounding areas. Furthermore, this preliminary study assesses the reliability of the proposed innovative methodology for modeling the heat source based on process temperature, offering a new alternative to the conventional approach of defining the geometric location of the heat flux.

Conclusions

This study presents a comprehensive comparison between two heat source models for laser surface treatment of Ti-6Al-4V, focusing on their ability to predict thermal fields and molten pool geometry (width and penetration depth). The two models under consideration - the conventional 3D conical Gaussian heat source and the elliptic paraboloid volumetric heat source - were both validated through a combination of numerical simulations and experimental data. The results indicate that both models provide stable and consistent predictions, but the elliptic paraboloid model offers superior accuracy, particularly in replicating the laser track profile. The findings underscore the importance of selecting an appropriate heat source model to achieve precise control over the laser treatment process. The elliptic paraboloid model, with its ability to more accurately simulate the elliptical nature of the laser spot, showed smaller discrepancies between the simulated and experimental results. This is crucial when surface functionalization is performed at the micro- and nanoscale, where even small variations in heat distribution can significantly impact the outcome. Additionally, this study highlights the potential of adopting a different technique for modeling heat sources based on process temperature rather than traditional geometric definitions of the heat flux. Future research will focus on integrating these models into real-world industrial applications, further refining the methodology to enhance its broader use in surface modification technologies. This will involve predicting phase evolution and corresponding mechanical changes, ultimately leading to a better understanding of how surface modifications influence the overall mechanical behavior of materials. Furthermore, the applicability of the system for a small scale application will be refined in order to assess the viability of the process for functionalizing the extruder cavity.

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