Modelling and numerical study of the effect of temperature rise in laser-induced darkening of mild steel

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Vishnu Narayanan[1], Kshitij Ghormode[1], Ramesh K Singh[1], Deepak Marla[1]

[1] *Department of Mechanical Engineering, IIT Bombay, Maharashtra, India*

Abstract

Surfaces processed by lasers are susceptible to oxidation. This causes a change in surface properties and also the appearance of the surface. This is undesirable in many applications such as laser cleaning and laser annealing. This work involves the development of a computational model to predict oxidation of the material during laser heating by accounting for both thermal effects and chemical kinetics. The thermal effects are captured using the OpenFoam software, and oxidation is predicted using Thermocalc software based on the thermal history. The temperature rise and the oxide formation during laser scanning at different laser powers were simulated and compared to experiments. The results indicate that between 31 – 36 W laser power, the heating rates can go up to 4.6×10^6 K/s and lead to the formation of wustite (FeO). The FeO content undergoes a minute decrease with the increase in laser power. The results were consistent with experimental observations.

Keywords: Laser scanning, computational model, oxidation.

1. Introduction

Laser surface processing is one of the important industrial applications of lasers [1]. An important phenomenon observed during the laser processing of mild steel is oxidation. This is an exothermic reaction and is hence desirable in many applications such as laser cutting. However, in many laser processes such as cleaning and annealing, it is imperative to have a good surface quality after processing. Oxidation darkens the mild steel surface and makes it aesthetically unappealing [2].

The effect of oxidation has been studied comprehensively by many researchers [2-6]. Ivarson et al. conducted a numerical study on the ignition-extinction cycle that occurs during laser cutting of mild steel [3]. A diffusion model was used to study the gradient of oxygen concentration inside the melt pool and its effect on the cutting process. Chen et al. developed a numerical model for oxygen assisted laser cutting of mild steel [4]. The model accounted for the oxidation rate and used it to calculate the reaction energy released by oxidation. A more in-depth analysis was done by Antonov et al., who used a standard solution of Wagner's problem to solve the governing equation analytically in 1 D and estimate the oxide layer thickness [5].

A recent work in numerical modelling was by Larsson et al. [6]. They developed a model using DICTRA, which is an add-on module for the commercial software Thermocalc and studied the kinetics of formation of different oxide phases on pure iron at a constant temperature. To the best of the authors' knowledge, not much study has been conducted in the formation of oxide content during laser processing of mild steel. Understanding the extent of oxidation, and the relative percentage of different oxides formed, as a function of laser power is necessary for applications such as laser cleaning and laser annealing. More knowledge of the oxidation process would help in selecting the optimum laser parameter for these applications.

This works aim at investigating the oxidation rates and oxide phases formed during laser processing of mild steel. The objective of this study was to develop a numerical model which would aid in the prediction of oxidation when a continuous wave (CW) laser is scanned over the surface of mild steel. A numerical model is developed, from which the laser heating and cooling rates during the process and the temperature profiles are obtained. With this information, the oxidation rates and relative concentrations of different iron oxides are estimated. Using the model, a direct correlation of the heating and cooling rates with oxidation of mild steel can be established and thereby predict the possibility of colouration at any parameter values. This model can be directly used to determine the possibility of colouration during applications such as laser annealing, welding etc. Section 2 describes the numerical model developed and the details of the experimental setup used for validation. The results of the numerical model and the experimental study are given in section 3, and its conclusions are in section 4.

2. Model description

The process of heating mild steel by a CW laser and the subsequent oxidation is studied numerically in this study. The absorption of the laser causes the metal to get heated to temperatures even higher than the melting point. High temperature accelerates the oxidation reaction and the diffusion of oxygen into the material. The rate of oxidation reaction would depend on the time rate of increase of temperature. The oxides formed could be hematite, magnetite or wustite. The colour observed in the laser-heated surface would depend on the oxide formed. Hence prediction of the type of oxide formed is necessary. To predict the formation of oxide, a model which accounts for the laser heating and the oxidation kinetics was developed. The details of the numerical modelling are given in the following subsections.

2.1. Laser heating

The numerical model for simulating the thermal processes was developed using open-source CFD software, OpenFoam. The model accounted for a laser source moving at a constant scan speed, heating and phase change. The geometry used for the simulation is shown in Fig 1. A 3-D geometry of size 300 μm × 200 μm × 2 μm was chosen for the study. The standard material properties of mild steel were assumed for the study. The material properties were assumed to be constant with temperature. The geometry was divided into hexahedral meshes of size 1 μm × 1 μm × 0.1 μm after conducting a grid independence study.

The main governing equation is the heat conduction equation [6].

$$K\nabla^2 T - \rho C_p \frac{\partial T}{\partial t} - \rho C_p u \nabla T = 0,$$

where K is the thermal conductivity of the material, ρ is the density of the material, C_p is the specific heat capacity of the material and u is the scan speed.

The optical penetration depth of steel for a wavelength of 1070 nm is around 10 - 20 nm. Therefore the energy input by laser was assumed as a surface heat flux. The laser heat source is accounted for by a moving heat flux at the top boundary with,

$$\ddot{q} = \frac{P}{\pi r^2} \; at \; z = 0 \text{ and } (x - ut)^2 + y^2 \le r^2,$$

where P is the laser power and r is the radius of the laser beam. All the other boundaries were assumed to be thermally insulated. The energy losses due to convection and radiation were found to be negligible compared to the laser power. So the effects of convection and radiation were neglected.

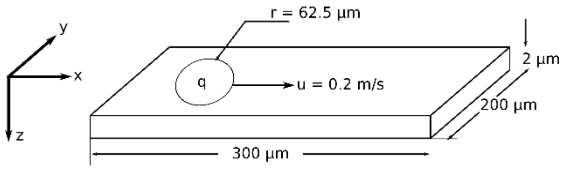

Fig 1: Schematic of the numerical model

2.2. Oxidation kinetics

When the material is heated with a laser, the material undergoes a chemical transformation. The high temperature leads to the ignition of metal causing the formation of iron oxides at the surface. There would be a change in the concentration of species leading to the diffusion of species. The high μtemperature would accelerate the diffusion of oxygen into the material volume, causing an increase in the thickness of the oxide layer. By calculating the transport property and flux of each species, the local molar volume of each species can be obtained. This would help in understanding the /growth of different oxide layers.

The numerical simulation was conducted in Thermocalc using the DICTRA module. The software models the thermodynamics and kinetics of each phase using mathematical expressions and experimental data. The flux of an element k is given by the equation

$$J_k = -M_k c_k \frac{\partial \mu_k}{\partial z},$$

where J_k is the flux of element k along the z-direction, M_k is the mobility, c_k is the concentration and μ_k is the chemical potential. The Thermocalc software contains a database of mobility for the FEO system. The concentration of species is calculated by numerically solving the equation of continuity which is given by

$$\frac{\partial c_k}{\partial t} = \frac{\partial(-J_k)}{\partial z}.$$

The databases FEDEMO, MFEDEMO and OXDEMO were used in this study. The formation of three different oxide phases (hematite, magnetite and wustite) were considered. A planar geometry was used with a grid size of 100 nm. The temperature rise with time was obtained from the thermal model described in the previous subsection. Using that data, the kinetics of the oxidation reaction was predicted and the amount of oxides formed was calculated.

2.3 Experiments

The experiments were conducted on mild steel samples using the laser equipment, IPG Photonics YLS-600/6000-QCW. It is a quasi CW solid-state multimode laser with a wavelength of 1070 nm. It operates in both CW and pulsed mode but was used in CW mode for the current study. It is scanned using a 5 axis CNC stage. The samples used were commercially available mild steel plates (AISI 1018). The samples were polished and cleaned before the experiments. In this study, the laser was operated at a constant scan speed of 200 mm/s and a beam diameter of 125 μm. According to the preliminary studies, the power values between 31 – 36 W raised the surface temperature above the melting point (1753 – 1799 K) and boiling point (3134 K) of mild steel. Therefore, for the study, the power was varied from 31 W to 36 W with a power increment of 1 W. The samples were analysed using an optical surface profilometer (Alicona Infinitefocus) after the laser scanning. The dimensions such as the width of the lines scanned and the relative height of processed and unprocessed regions was studied using the profilometer.

3. Results and Discussion

3.1. Temperature rise during laser processing

Figure 2 shows the temperature distribution on the metal surface at a given instant and Fig 3 shows the variation in maximum temperature at the surface at different laser power values. The maximum temperature attained is directly proportional to the laser powers. Since the laser is multi-mode the temperature will be close to the maximum temperature for almost the entire beamwidth. The results show that the laser power between 31-36 W can heat the material above the melting point (1753-1799 K). The maximum temperatures are not high enough to cause material removal. The width of the melt pool and heat affected zone was obtained

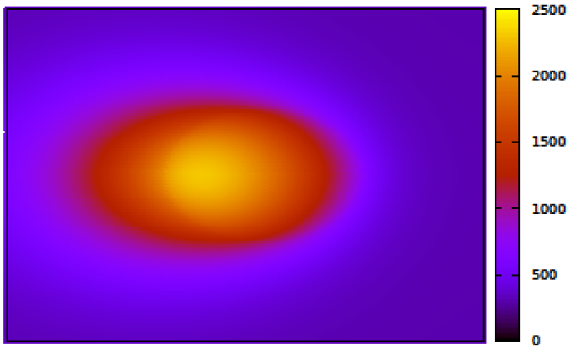

Fig 2: Temperature contour at time, t = 0.5ms

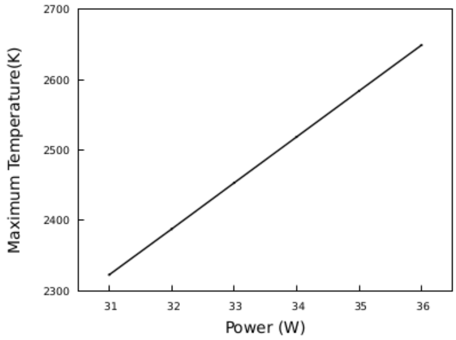

Fig 3: Maximum temperature attained at different laser power

from these results and were compared with experimental observations for the validation of the model.

3.2. Heating rates during laser processing

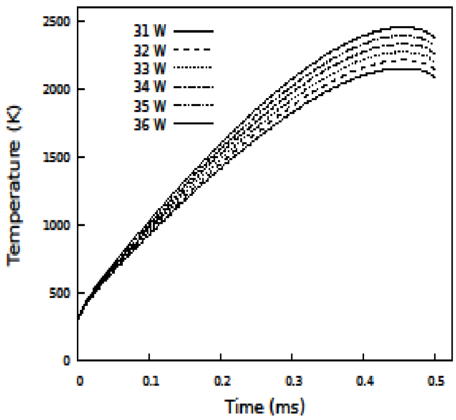

Fig 4: Heating rates at different laser power

Figure 4 shows the increase in temperature with time at different laser powers. The heating rates influence the chemical changes that occur in the material surface. Due to the constant scanning speed and laser beam diameter, the temperature values reach the peak at the same instant of time for all the power values. It can be observed that the heating rates increase from around 4.6 × 10^6 K/s to 5.9 × 10^6 K/s in the power range between 31 – 36 W. The heating rates are quite high and will cause oxidation of the surface. The difference in heating rates is significant and would affect the kinetics of the oxidation reaction. Therefore the oxide content can be expected to be different for 31 W and 36 W.

3.3. Oxidation rates v/s power

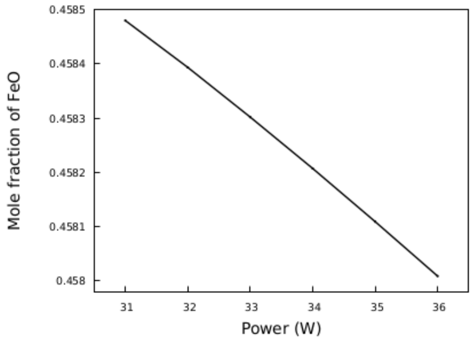

Fig 5: Mole fraction of wustite at different laser power

Figure 5 shows the variation of mole fraction of oxide at a layer of 1 μm thickness at the surface of the material with an increase in power. The heating rates obtained from the thermal model were used to identify the formation of the oxide layer and the composition of various oxides in the layer. The study considered the formation of three different iron oxides, wustite (FeO), hematite (Fe_2O_3), and magnetite (Fe_3O_4). Wustite and magnetite are black in colour whereas hematite is red in colour. The results of the simulation showed the formation of only wustite. The simulation did not show any formation of hematite or magnetite. It was observed that the mole fraction of wustite reduced with an increase in power. The reduction in wustite content is negligible. Therefore the results suggest that the laser would lead to darkening of the material at all powers between 31 – 36 W. The results also suggest that there could be a slight decrease in the darkening effect when power is increased from 31 W to 36 W.

3.4. Variation in colour with laser power

Figure 6 shows the surface of mild steel after laser scanning at different powers. The results of the experimental study were used to validate the model. The width of the melt pool was measured using Alicona Infinitefocus. Figure 7 shows the comparison of experimental and computational results of the width of the melt pool. It was observed to be close to the value predicted by the thermal model with a

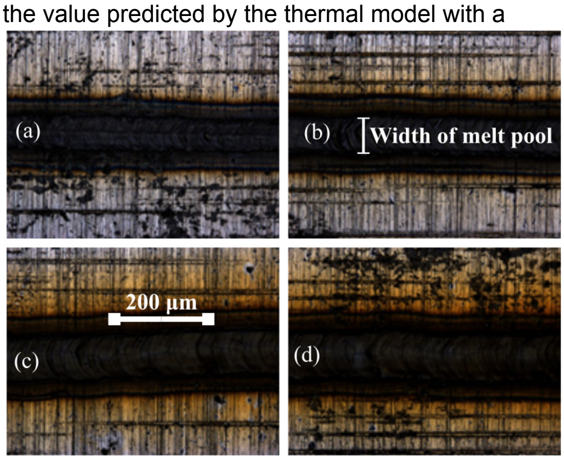

Fig 6: Surface after laser scanning at (a) 32 W, (b) 34 W, (c) 35 W and (d) 36 W

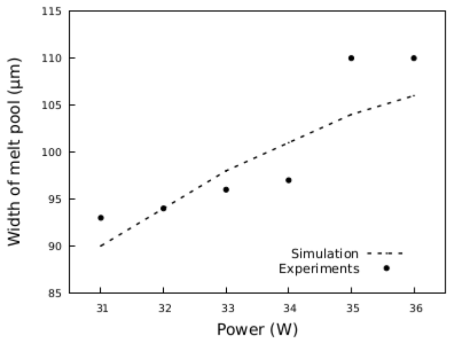

Fig 7: Width of melt pool at different laser powers

discrepancy of around 4 %. As predicted by the model,
the surface had effects of melting and darkening for all powers used in the study. The 3-D surface profile showed no craters or signs of material removal at any of the power values.
It can be observed that the mild steel surface appears darker at lower powers and develops a brownish shade as the power is increased. This is supported by Fig 8 which shows the variation in colour values (% RBG) with power.

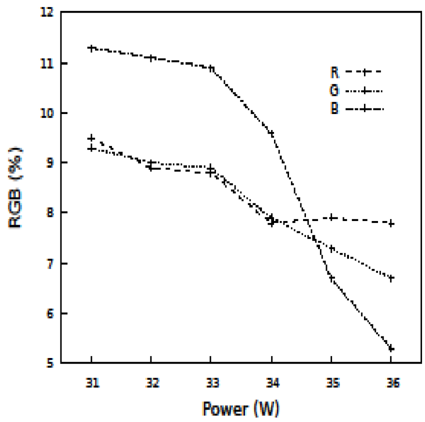

Fig 8: Colour values of the oxide layer at different powers

The results suggest that the black coloured iron oxides (wustite or magnetite) are the major oxide at the powers used in the study. The formation of brown colour suggests the formation of hematite or maghemite. The negligible change in colour values below 34 W indicates that the presence of hematite or maghemite is negligible at that power. As the power is increased, the red-brown coloured oxides start forming. However, the black coloured oxides are still the major component at the surface at laser power values. The experimental observations align with the results of the numerical model.

5. Conclusions

The work presented a computational model for simulating laser heating of a mild steel surface and the chemical changes that follow it. The model predicts the heating of the surface and the extent of oxide formation at various laser powers. The model can be used to study the chemical transformation during laser scanning at various parameter values. Few notable observations that were made from the results of the study are

- At the given parameter values, the temperature is sufficient to melt the material but insufficient to cause material removal.
- The time rate of change of temperature varies from 4.6×10^6 K/s to 5.9×10^6 K/s with an increase from 31 W to 36 W.
- The oxide content decreases slightly with an increase in power.
- The powers between 34-36 W would cause the formation of hematite.

It can be concluded that the model could predict with some accuracy the oxidation process during laser scanning. The model can be used to determine whether the chosen parameter values would lead to oxidation and darkening of the surface.

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