Development and Application of Three-Dimensional Numerical Model for Characterization of Thermal Fields during Surface Laser Treatment of Solid Materials

V. Antonov\textsuperscript{1}, I. Iordanova\textsuperscript{2},
\textsuperscript{1}Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, 72 Tzarigradsko chaussee Blvd., Sofia 1784, Bulgaria
\textsuperscript{2}Department of Solid State Physics and Microelectronics, Faculty of Physics, University of Sofia, 5 J. Bouchier Blvd., Sofia 1164, Bulgaria

Received 6 June 2008

Abstract. The finite elements method (FEM) with cylindrical symmetry was developed for solving the three-dimensional differential heat transfer equation. The method was applied for the characterization of the temperature field created in low carbon sheet steel during its surface laser treatment with Nd:Glass pulsed laser. The influences of the temperature dependences of the material thermal properties and the energy distribution across the laser beam have been analyzed. A comparison with the results obtained by the frequently used one-dimensional FEM was performed.

PACS number: 44.05.+e; 42.62.Cf

1 Introduction

Laser processing is a prospective method for materials properties improvement based on the local heating caused by the optical absorption of laser radiation. Surface laser treatment of solid materials is used at present for modification of microstructure and a number of physical, mechanical and other macroproperties. The parameters change of the treated materials is mainly due to the created in them thermal fields. That is why the characterization of these fields is of great importance for the understanding and governing the processes taking part during surface laser treatment and thus for the achievement of an efficient modification of the materials properties.

The induced by the laser irradiation heating can be described by the heat conduction equation. It is a three-dimensional partial differential equation, the solution
of which can be realized either by analytical or by numerical methods, as for example finite elements methods (FEM).

Contrary to the analytical method, by the FEM the temperature dependence of properties and the energy distribution across the laser beam can be considered. In general, for the realization of numerical methods the volume of the investigated material is represented as a system of small elementary volumes. According to the Fourier heat conduction theory the heat transfer flux through a given plane of the element is a function of the temperature gradient in that plane. The temperature gradient is assumed constant in the element and thus higher order terms are neglected. Besides the above mentioned advantages, by the FEM the effects of size and geometry and heat transfer through the boundaries can be taken into account.

This study is related to our former paper [1], in which the analytical and one-dimensional FEM have been adopted and applied for the characterization of thermal fields in low-carbon rimming sheet steel during its surface laser treatment with pulsed Nd:Glass laser. In the present paper our achievements in the development and application of the three-dimensional FEM for the characterization of the same steel exposed to laser treatment are presented.

2 Experimental Part

2.1 The heat diffusion equation

According to [2–4] the heat equation corresponding to the temperature field created in the material during surface laser treatment can be represented as follows:

\[
\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} (K \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (K \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z} (K \frac{\partial T}{\partial z}),
\]

where \(x, y, z\) are the coordinates, \(T\) is the temperature, \(t\) – the time, \(K\) – the thermal conductivity coefficient, \(W\) – the power of the heat source (laser beam), \(\rho\) – the physical density of the treated material, and \(c\) – specific heat capacity.

When the relation \(r_0 \gg (k \tau)^{0.5}\) is fulfilled (where \(r_0\) is the radius of the laser spot, \(k = K/(\rho c)\) – the thermal diffusivity, \(\tau\) – the laser pulse duration, and \((k \tau)^{0.5}\) – the thermal diffusion length), equation (1) could be simplified to one-dimensional [2–4]. This assumption is useful for the most practical applications. However, as demonstrated in [1], when the relation \(r_0 \gg (k \tau)^{0.5}\) is not fulfilled the original three-dimensional equation heat transfer should be solved. This is usually the case when the beam radius is very small, the pulse duration is relatively long or the material thickness is comparable to the thermal diffusion length.
2.2 Description of the numerical finite elements method (FEM) used for the heat diffusion equation solution

The developed in the present study FEM method for solution of the heat conduction differential equation is based on Refs. [2, 3]. Cylindrical symmetry of the problem is used. The beginning of the coordinate system is in the centre of the laser beam. The way of separation of the samples volume in cylindrical elements is represented in Figure 1.

![Figure 1. Scheme of the elements for the FEM.](image)

The coordinates \((r, z)\) of each element are defined as it is shown in Figure 1 and the temperature \(T\) is assumed constant in all the space of a particular element. The temperature change versus time is characterized via the following iteration formula:

\[
T_{i,j}(t + \Delta t) = T_{i,j}(t) + k \left( \frac{T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4T_{i,j}}{\Delta r^2} + \frac{T_{i+1,j} + T_{i-1,j}}{2r\Delta r} \right) \Delta t, \tag{2}
\]

where \(\Delta t\) is the time step, and \(i, j\) denote the index numbers of a particular element.

The evaluations via the developed three-dimensional FEM were realized by the created program code, written in PASCAL language. The space step was \(\Delta r = 5 \times 10^{-6} \text{ m}\) and the time step \(\Delta t = 5 \times 10^{-8} \text{ s}\). The initial temperature in the body was accepted to be \(T_0 = 20^\circ\text{C}\). According to the assumptions in Refs. [3, 5, 6] and the results from our previous investigations [1] isolated borders boundary conditions were applied, described by the following equation:

\[
K \frac{\partial T}{\partial z} = 0. \tag{3}
\]

In the developed and applied FEM method the calculations were performed both with and without consideration of temperature dependence of material properties. The distribution of energy across the laser beam section was modelled by
the Gaussian \( F(x, y, z) = \exp \left\{ -\frac{x^2 + y^2 + x^2}{r_0^2} \right\} \) and homogeneous function \( F(x, y, z) = 1, (x^2 + y^2 + x^2 \leq r_0^2) \cap F(x, y, z) = 0, (x^2 + y^2 + x^2 > r_0^2) \). The evolution of the laser power in time is taken as those of a pulse with duration \( \tau \):

\[ \Theta = 1, (t \leq \tau) \cap \Theta = 0, (t > \tau). \]

Results were compared with the obtained by the one-dimensional heat equation, presented in [1].

2.3 Description of the analyzed surface laser treated material

Material parameters used for the thermal field simulations correspond to those of 08kp (low carbon rimming) sheet steel (with two thicknesses namely \( d = 0.45 \text{ mm} \) and \( d = 2.5 \text{ mm} \)), whose modified microstructure and hardness due to its surface treatment by Nd:Glass pulsed laser have been analyzed in our former papers [7–9].

The used for the present simulations values of the physical density, thermal conductivity and specific heat capacity have been taken from [10] and are as follows: \( \rho = 7800 \text{ kgm}^{-3} \), \( K = 33 \text{ Wm}^{-1} \text{ K}^{-1} \), \( c = 650 \text{ Jkg}^{-1} \text{ K}^{-1} \). The absorption coefficient \( A \) has been measured by NKD-8000 spectrometer and evaluated as \( A = 0.4 \). The temperature dependencies of the specific heat capacity \( c \) and thermal conductivity \( K \) have been considered via an interpolation performed over a number of reference data points, as it was shown in [1]. The laser beam parameters are equivalent to those used in [7–9] and are as follows: pulse energy \( E = 6 \text{ J} \), the laser pulse duration \( \tau = 7 \text{ ms} \), radius of the laser beam \( r_0 = 1 \text{ mm} \). The initial temperature of the body was accepted to be \( T_0 = 20 \text{°C} \).

3 Results and Discussion

Figure 2 represents the results for surface temperature change during and after the laser pulse obtained by the created three-dimensional FEM. The evaluated temperatures correspond to the center of the laser spot. The calculations have been performed by considering and neglecting the temperature dependence of thermal conductivity and thermal capacity and by assuming homogenous and Gaussian intensity distribution.

The results show that the consideration of temperature dependence of the material properties leads to an increased speed of heating and to a decrease of the cooling rate after the end of the pulse in respect to the values obtained assuming constant thermal properties. The maximal achieved surface temperature slightly depends on the consideration of temperature dependence of thermo-physical properties (the differences between the two obtained values are less than 1%). The curves in Figure 2 corresponding to the case of temperature dependent material properties (particularly for the Gauss distribution) show gradient changes on their rising and falling parts. These changes, observed around 720° C reflect the reversible polymorphous ferrite \( \leftrightarrow \) austenite transformation which for
Development and Application of Three-Dimensional...

Figure 2. Influence of the temperature dependence of the material properties on the surface temperature in the center of the laser spot.

- a) thickness $d = 2.6$ mm
- b) thickness $d = 0.45$ mm
the analysed steel occurs in this temperature interval. Thus, the approach with considering the temperature dependence of the properties is closer to the real situation. The introduction of temperature dependent heat capacity consideration affects the heating and cooling velocities only and does not change the value of the maximum achieved surface temperature.

It is also obvious that for both cases of constant and not constant properties the plots corresponding to the Gauss distribution of energy have greater rates of heating and cooling and the corresponding maximal achieved temperature is with about 10% higher than that for the homogenous intensity distribution. For the former case the energy is more concentrated around the center of the laser beam which at the initial stages of treatment causes higher heating rate and consequently after the end of the pulse increases the cooling rate as well.

In Figure 3 results for the temperature field distribution on the surface versus time are presented. No dependence of the temperature distribution on the thick-
ness is observed. The heat affected zone (HAZ) on the surface is limited by the radius of the laser spot, i.e. $r_0 = 1$ mm. Thus, in order to prevent the overlapping of the laser spots on the surface the distance between their centers should be at least equal to the diameter of the laser beam. The consideration of the temperature dependence of the material’s properties results in an increase of the surface HAZ and of the heating and cooling rates. The maximal surface temperature is achieved considering Gaussian energy distribution but in this case the HAZ is higher compared to the case of homogenous distribution. The rate of temperature decrease versus the distance from the centre is almost constant.

For the case of homogenous energy distribution the situation is completely different. The decrease of temperature within a region defined by the heat diffusion length $D_h = 2(k, \tau)^{0.5} = 0.426$ mm is not more than 10% from the maximal temperature in the centre of the spot. After this distance the temperature quickly falls to that of surrounding bulk. Homogenous distribution corresponds to the
multimode laser beam and from the results it can be concluded, that this type of intensity distribution should be used for surface treatment of the materials in order to obtain better results.

Figure 4 and Figure 5 represent the simulated temperature change in depth of the steel plates due to the applied surface laser treatment. The results show that the consideration of the temperature dependent properties leads to an increase of the surface temperature values (with maximum 15%) and to a decrease of the cooling rate after the end of the pulse in respect to the values obtained assuming constant thermal properties. Although the introduction of the temperature dependent heat capacity consideration does not change the maximum achieved surface temperature, this consideration affects the heating and cooling velocities during and after the laser pulse. In the curve plotted for the case considering the temperature dependencies of both the thermal conductivity and heat capacity a gradient change on the rising and falling parts at temperature $\sim 720^\circ$C corre-
Figure 4b. Temperature change in the depth under the center of laser beam of steel plates for the time period equal to double time of the pulse duration (thickness $d = 0.45 \text{ mm}$).

The results point out that the way of considering materials thermal properties affects more significantly the temperature change in depth than the temperature on the surface. For the case of temperature dependent thermal conductivity the temperature in depth for each of the two materials (thick and thin) increases faster than the observed for the case of constant thermal properties. Thus considering the temperature dependence of thermal conductivity results in an effectively increased HAZ in the material. These results give the same dependencies as for the one-dimensional model, presented in [1] and also are similar with the results for the surface HAZ. Due to the heat transfer to the surrounding bulk of the material the influence of the heat reflection from the opposite to the laser treated surface is less important than it has been found for the one-dimensional
Figure 5. Temperature change in the depth under the center of laser beam of steel plates with thickness 0.46 mm for the time period equal to ten times laser pulse duration.

case [1]. The temperature field in the depth of the material shows dependence on the intensity distribution in the laser spot. The HAZ is smaller for the Gaussian distribution regardless the temperature dependence on the thermophysical properties and thickness. For the surface temperature distribution as it was mentioned this could be due to the concentration of energy near the centre of the laser beam. From these results it can be concluded that the most suitable for material treatment is laser beam with homogenous intensity distribution.

The previously observed effects in [1] of the material thickness influence on the temperature field are also visible in Figure 5. It is obvious that for the thin material the temperature in depth increases faster than in the thick one although in lesser degree than the observed applying the one dimensional model. The temperature in the time interval between 25 and 140 ms tends to become constant in depth. This abnormality is assumed to be due to the low thickness, being
comparable with the thermal diffusion length. Due to the heat transfer to the surrounding bulk the temperature decreases in the same rate regardless the depth. Contrary to that in the case of one-dimensional model the temperature remains constant in time [1], which makes the one-dimensional model unsuitable for the characterization of thermal fields in this material.

4 Conclusions

1. A three-dimensional finite elements method (FEM) with cylindrical symmetry has been developed and applied for the characterization of thermal field arising in mild sheet steel plates with two different thicknesses during their surface treatment with Nd:Glass laser.

2. The influence of the temperature dependence of thermal properties on the parameters of thermal field has been analyzed. The results show that this influence is not strong when the maximum surface temperature is concerned but it is significant for the parameters of the heat affected zone in depth.

3. Opposite to the one-dimensional case the developed FEM three-dimensional models are applicable for the analysis of temperature field in depth of materials with thickness smaller or comparable with their heat diffusion length \((k \cdot \tau)^{0.5}\).

4. Assuming Gaussian intensity distribution of intensity in simulations gives higher maximal achieved temperature, but the HAZ in the surface and in depth is less than when the homogenous intensity distribution is assumed.

5. In order to achieve more uniform and localized level of properties modification multimode laser beam with homogenous energy distribution should be used.

Acknowledgments

The authors would like to acknowledge the financial support from Marie-Currie foundation and from the Scientific Funds at the Ministry of Education and Research, Bulgaria (project No VUF 07/05) and at Sofia University (Project No 98/2008).

References

V. Antonov and I. Iordanova