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

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Abstract. The finite elements method (FEM) was developed for solving the one-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 dependencies of the material thermal properties, the convective and radiative heat transfer and the finite size of the treated object have been analyzed.

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1 Introduction

Laser processing is a prospective method for materials properties improvement based on the local heating caused by the optical absorption of the laser radiation. Surface laser treatment of solid materials is used at present for the modification of microstructure and a number of physical, mechanical and other macro-properties. Because the parameters change of the treated material is mainly due to the thermal field created in it the characterization of this field is of great importance for the understanding and governing the processes during the surface laser treatment.

The heating caused by the laser irradiation can be described by the heat conduction equation. It is generally a three-dimensional partial differential equation, the solution of which can be realized either by analytical or by numerical methods. For the particular cases when the diameter of the laser beam is more than

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five times larger than the heat diffusion length, the heat conduction equation simplifies to one-dimensional [1–3].

Analytical methods assume temperature independent material properties, regular geometry and negligible heat losses due to convection and radiation. These methods are simple to be performed and are widely used for the thermal field evaluations [4–8].

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 the higher order terms are neglected. The main advantage of these methods also called finite element methods (FEM) is the possibility to take into account the temperature dependence of the material properties, effects of size and geometry and heat transfer through the boundaries. However, in some cases the FEM are slower than the analytical methods [2, 9–11].

This paper represents an analysis of the temperature distribution in a body subjected to laser irradiation. One-dimensional heat conduction equation has been used for the characterization of the thermal field created in low carbon mild sheet steel during its surface laser treatment by Nd:Glass pulsed laser. In the developed for the purposes of the present investigation numerical FEM method the temperature dependence of the properties, boundary heat losses and thickness of the treated material were taken into account.

2 Experimental Part

2.1 The heat diffusion equation

According to [1–3] the heat equation corresponding to the temperature field created in the material during surface laser treatment can be represented as follows:

$$\rho c\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}(K\frac{\partial T}{\partial x}) + \frac{\partial}{\partial y}(K\frac{\partial T}{\partial y}) + \frac{\partial}{\partial z}(K\frac{\partial T}{\partial z})\,, \tag{1}$$

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

When the relation $r_0 \gg (k\tau)^{0.5}$ is fulfilled, (where r_0 is the diameter of the laser spot, $k = K/(\rho c)$ – the thermal diffusivity, τ is the laser pulse duration, and $(k\tau)^{0.5}$ – the thermal diffusion length) the one-dimensional heat transfer equation (2) is applicable [1–3]:

$$\frac{\partial^2 T(z,t)}{\partial z^2} - \frac{1}{k}\frac{\partial T(z,t)}{\partial t} = -\frac{W(z,t)}{K}\,. \tag{2}$$

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 information taken from for one-dimensional case [2, 9, 10]. The line space has been divided into small elements with a linear size Δr and temperature T in the center of the element. For the temperature change estimation as a function of time the following iteration formula with a time step Δt has been used:

$$T_i(t+\Delta t) = T_i(t) + k\Big(\frac{T_{i+1} + T_{i-1} - 2T_i}{\Delta r^2}\Big)\Delta t\,, \tag{3}$$

where i denotes the index number of a particular element.

The surface temperature T_S has been evaluated by a second order interpolation of the corresponding temperatures to the three closest to the surface elements:

$$T_S = \frac{1}{8}(15T_1 - 10T_2 + 3T_3), \tag{4}$$

where T_1, T_2, and T_3 are the temperatures of the three closest to the surface elements, ordered by increasing distance from the surface.

The connection between the depth z and the element index number i obeys the following equation:

$$z = i\Delta r\,. \tag{5}$$

The evolution of the laser beam intensity in time follows the equation:

$$I_0 = \frac{E}{\tau\pi\frac{r_0^2}{4}}, \qquad (t \le \tau) \cap I_0 = 0,\ (t > \tau), \tag{6}$$

where E denotes the energy of the laser pulse, τ – the duration of the pulse, and A is the coefficient of the optical absorption of the laser radiation in the treated material.

In the present study for the evaluations *via* the FEM method a program code, written in PASCAL was created. The space Δr and the time Δt steps used for the simulations were $\Delta r = 5 \times 10^{-6}$ m and $\Delta t = 5 \times 10^{-8}$ s, respectively. The initial temperature in the body was accepted to be $T_0 = 200$°C. Similarly to the models used in [1, 13] the calculations were performed for the following two boundary conditions:

— isolated borders, for which case the following equation is valid:

$$K\frac{\partial T}{\partial z} = 0\,; \tag{7}$$

— convective heat transfer through the borders described as follows:

$$K\frac{\partial T}{\partial z} = h(T - T_0)\,, \tag{8}$$

where h is the convection coefficient.

Using the methodology for horizontal plates described in [13] it was calculated that independently on the material or thickness on the plates surface $h = 24\ \mathrm{W\,m^{-2}K^{-1}}$, while on its bottom part $h = 11\ \mathrm{W\,m^{-2}K^{-1}}$.

— radiative heat transfer described by the equation:

$$K\frac{\partial T}{\partial z} = A.\sigma(T^4 - T_0^4)\,, \tag{9}$$

where $\sigma = 5.67051 \times 10^{-8}\ \mathrm{W\,m^{-2}K^{-4}}$ is the Stephen-Boltzman constant [1, 13] and A is the coefficient of the optical absorption of the laser radiation (0.4 for low carbon steel) [2, 3, 14].

2.3 Description of the analyzed surface laser treated material

Material parameters, used for the thermal field simulations correspond to those of 08kp sheet steel (with two thicknesses namely $d = 0.45$ mm and $d = 2.5$ mm), whose modified microstructure and hardness due to its surface treatment by Nd:Glass pulsed laser have been analyzed in our former papers [15–17].

The used for the present simulations values of the physical density, thermal conductivity and specific heat capacity have been taken from [18] and are as follows: $\rho = 7800$ kg/m^3, $K = 33\ \mathrm{W\,m^{-1}K^{-1}}$, $c = 650\ \mathrm{J\,kg^{-1}K^{-1}}$. 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, taken from [18,19]. The analytical interpolation functions are given in Tables 1 and 2, and in Figures 1 and 2, the corresponding

Table 1. Interpolation function of the thermal conductivity K dependence based on data from [18]

Temperature range	Interpolation function for $K(T)$, $\mathrm{W\,m^{-1}K^{-1}}$
$273^\circ\mathrm{K} \le T \le 800^\circ\mathrm{K}$	$114.6667 - 0.0917T$
$T > 800^\circ\mathrm{K}$	33

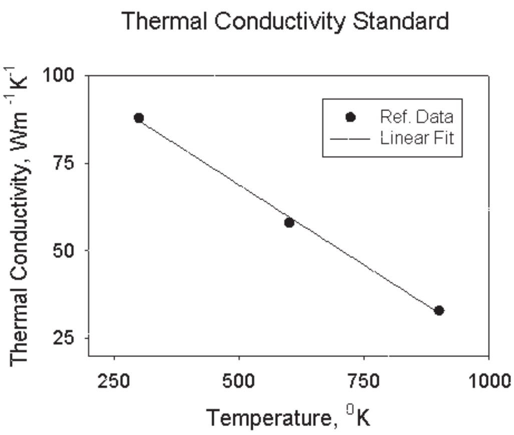


Figure 1. Interpolated temperature dependence of the thermal conductivity. The reference data are taken from [18].

Table 2. Interpolation function of the specific heat c based on [19]

Temperature range	Interpolation function for $c(T)$, $\mathrm{J\,kg^{-1}K^{-1}}$
$273°\mathrm{K} \le T \le 990°\mathrm{K}$	$284.7217 + 0.5051T$
$990°\mathrm{K} \le T \le 1089.5°\mathrm{K}$	$784.8746 + 3653.0135\exp\Big[-0.5\Big(\frac{\ln(T/1022.7773)}{0.0088}\Big)^2\Big]$
$1089.5°\mathrm{K} \le T \le 1123°\mathrm{K}$	$-12212.8643 + 11.9301T$
$T > 1123°\mathrm{K}$	1184.643

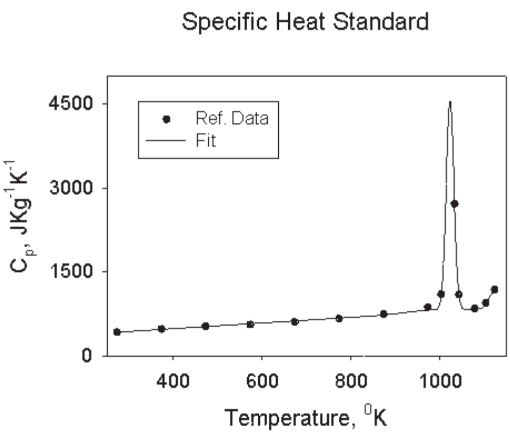


Figure 2. Interpolated temperature dependence of the specific heat. The reference data are taken from [19].

plots are represented. The peak at 1000 K (727°C) in Figure 2 is related to the occurring in the treated steel at this temperature polymorphous *ferrite* $\rightarrow$ *austenite* transformation. The laser beam parameters are equivalent to those used in [15–17] and are as follows: pulse energy $E = 6$ J, the laser pulse duration $\tau = 7$ ms, diameter of the laser beam $r_0 = 2$ mm.

3 Results and Discussion

3.1 A case of material with temperature independent properties

Firstly some preliminary calculations have been performed for the case of thermally isolated borders. The used for these simulations thickness of the steel is 2.6mm, which is significantly higher than the corresponding thermal diffusion

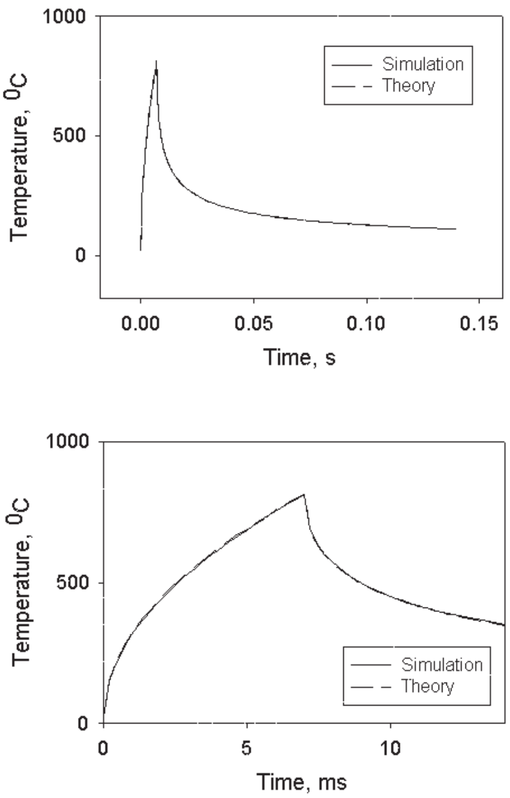
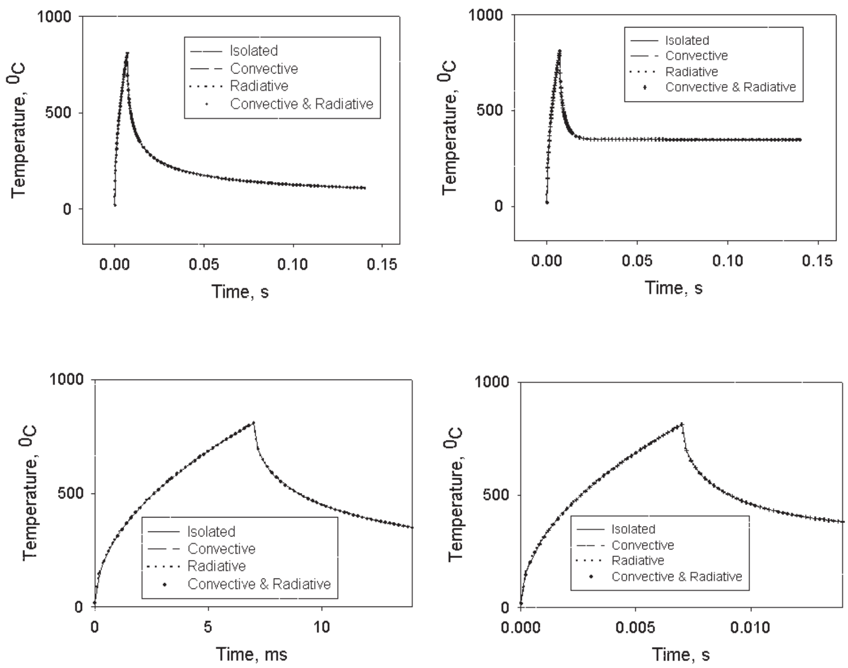


Figure 3. Surface temperature versus time for semi-infinite body (mild sheet steel with thickness 2.6mm) with thermally independent properties, estimated with analytical (theory) and numerical FEM (simulation) methods.

length ($(k\tau)^{0.5} = 0.213$ mm). Thus, the body can be assumed as a semi-infinite in size. The results for the surface temperature estimated by the developed FEM together with the theoretical results obtained for a temperature independent material properties are represented in Figure 3. The difference between the two curves is less than 1% which proofs the accuracy of the developed FEM.

Then the influence of the heat transfer losses has been investigated at the following boundary conditions: thermally isolated border, convective heat transfer, radiative heat transfer, radiative and convective heat transfer.

Figure 4 represents the obtained according to equations (7-9) results for the temperature change at the surface of the two steel plates with a thickness of 2.6 mm (a) and 0.45 mm (b). The rising part of the plots corresponds to the heating during the laser pulse while the falling part reflects the cooling stage after the end of the laser pulse. It is obvious that the results obtained by the four considered boundary conditions are very similar. The evaluated differences between the surface temperature values for the above four cases are less than 1%. This is probably due to the fact that the heat transfer due to convection and radiation is smaller compared to that due to the heat conduction inside the material. Thus,



a) thickness $d = 2.6$ mm　　a) thickness $d = 0.45$ mm

Figure 4. Surface temperature change calculated by FEM for different boundary conditions represented in two different x-scales.

it can be concluded that the simplest case of isolated material borders can be a good approximation for the evaluation of the surface temperature change during the applied surface laser treatment.

From the two top graphs in Figure 4 it is obvious that the cooling of the thinner sample occurs slower. Within the analyzed time interval its temperature during the cooling stage stays higher than that of the thicker plate. For the former sample within the interval between 25 and 140 ms the surface temperature is practically constant while for the latter it continually decreases. The slowed cooling of the thinner sample whose thickness (0.45 mm) is close to that of the thermal diffusion length (0.213 mm) could be related to the reflection of the heat current from the opposite to the laser treated side back into the material. Because of the much higher thickness of the thicker sample (2.5 mm) this effect would be negligible.

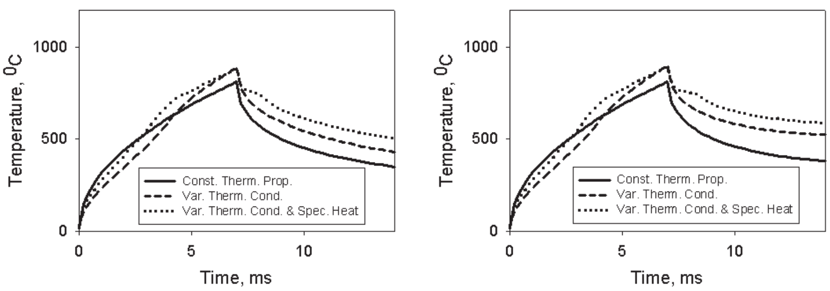
3.2 A case of material with temperature dependent properties

The numerical experiments by the developed FEM for this case have been performed for the following two cases:

— temperature dependent thermal conductivity, constant heat capacity;

— temperature dependent thermal conductivity and heat capacity.

The temperature dependent parameters have been evaluated according to the interpolation functions represented in Tables 1 and 2 and in Figures 1 and 2. The obtained for the last two cases results for the surface temperature change due to the applied surface laser treatment together with those for the case of constant thermal properties are represented in Figure 5.



a) thickness $d = 2.6$ mm   a) thickness $d = 0.45$ mm

Figure 5. Influence of the temperature dependence of the material properties on the surface temperature.

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 $\sim 720^0C$ corresponding to the reversible polymorphous $ferrite \leftrightarrow austenite$ transformation during the heating and cooling stages is observed. This result shows that from the three analyzed cases, the last one is the best approach to the real processes taking part in the steel during the applied surface laser treatment.

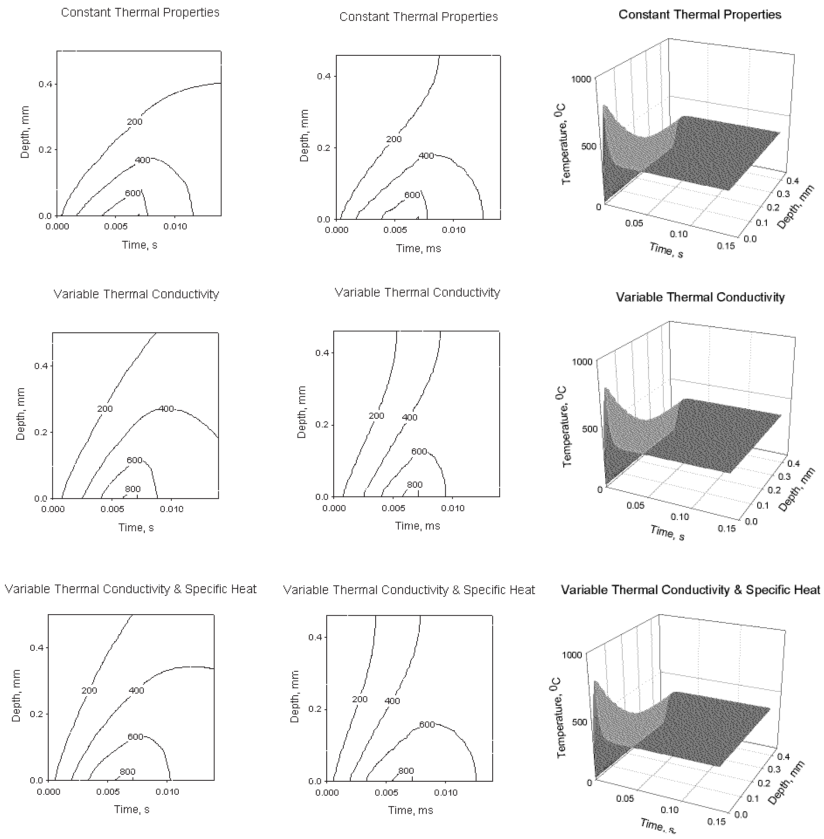
3.3 Analysis of the temperature change in the depth of the steel samples

Figure 6 represents the simulated temperature change in the depth of the steel plates due to the applied surface laser treatment.

The results show that the way of considering materials thermal properties affects more significantly the temperature change in the depth than the temperature on the surface. For the case of temperature dependent thermal conductivity (the plots in the second row of the graph), the temperature in depth for each of the two materials (thicker and thinner) increases faster than the observed for the case of constant thermal properties (see the first raw plots). Thus, considering the temperature dependence of thermal conductivity results in an effectively increased heat affected zone (HAZ) in the material. The additional consideration of the temperature dependent specific heat capacity (the third raw plots in the graph) causes a further increase of the HAZ. According to the obtained results for the last case, which is the closest to the real situation, it seems that the reflection of the heat from the opposite to the laser treated side probably occurs in the thicker material as well. This may be due to the effectively increased thermal diffusion length for the case when during the performed simulations the temperature dependencies of both thermal conductivity and specific heat capacity have been considered.

The previously observed effects of the material thickness influence on the temperature field are also visible in Figure 6. For example, in the thinner material the temperature in the depth increases faster than in the thicker one. It should be noted that in the performed in the present study simulations it has been assumed that the thermo-physical properties of the two referent samples are identical and isotropic.

In Figure 6c three-dimensional plots of the temperature change in the thinner material are represented. It is obvious that similarly to the results shown in



a) b) c)

Figure 6. Temperature change in the depth of steel plates; a) thickness $d = 2.6$ mm b) thickness $d = 0.45$ mm c) surface plot for thickness $d = 0.45$ mm

Figure 4 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 of this sample, being comparable with the thermal diffusion length, for which case the FEM seems to be not very suitable.

4 Conclusions

1. A one-dimensional finite elements method (FEM) for the evaluation of the thermal field created in materials during surface laser treatment has been developed and applied to a mild sheet steel plates with two d ifferent thicknesses (0.45 mm and 2.5 mm).

2. The influence of the heat losses due to convection, radiation and combined radiation and convection on the temperature field has been analyzed. It has been found that this influence is negligible and may be neglected.

3. The influence of the temperature dependence of the material's thermal properties on the created thermal field during the applied surface laser treatment has been analyzed. The results show that this influence is not significant when the maximum achieved surface temperature is concerned. However, the depth of the heat affected zone is strongly affected by it.

4. It has been shown that the developed FEM one-dimensional models are not applicable for the analysis of temperature field in the depth of materials with thickness smaller or comparable with their heat diffusion length ($(k\tau)^{0.5}$). However, the developed FEM method can be successfully used for the estimation of surface temperature of the materials whose thickness is comparable with $(k\tau)^{0.5}$ value.

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