TEMPLUM: A Process Adapted Numerical Simulation Code for The 3D Predictive Assessment of Laser Surface Heat Treatments in Planar Geometry

A. GARCÍA-BELTRÁN[1], J. L. OCAÑA[2] and C. L. MOLPECERES[2]
[1]Departamento de Automática, Ingeniería Electrónica e Informática Industrial – Centro Láser UPM
[2]Departamento de Física Aplicada a la Ingeniería Industrial – Centro Láser UPM
Universidad Politécnica de Madrid
ETSI Industriales, C/José Gutiérrez Abascal, 2. 28006 – MADRID
SPAIN
{agarcia, jlocana, cmolpeceres}@etsii.upm.es http://www.upmlaser.upm.es

Abstract: - A process adapted numerical simulation code for the 3D predictive assessment of laser heat treatment of materials has been developed. Primarily intended for the analysis of the laser transformation hardening of steels, the code has been successfully applied for the predictive characterization of other metallic and non metallic materials posing specific difficulties from the numerical point of view according to their extreme thermal and absorption properties. Initially based on a conventional FEM calculational structure, the developed code (TEMPLUM) reveals itself as an extremely useful prediction tool with specific process adapted features (not usually available in FEM heat transfer codes) in the field of laser heat treatment applications

Key-Words: - Numerical analysis; Finite element; Modeling; Simulation; Heat conduction; Laser surface treatments; Transformation hardening; Optical glass polishing

1 Introduction

Several valuable numerical simulation codes have been developed for the solution of different problems in the field of laser matter interaction at moderately high intensities leading to material transformation or phase changes. Mazumder and Steen [1] developed a numerical quasi-stationary 3D finite element model for the prediction of laser material processing with consideration of temperature dependent material properties and convection and radiation losses. Fritsch and Bergmann [2] developed a combined 2D-3D finite element model for the study of carbon diffusion during the transformation heat treatment of steels. Kechemair [3] developed a two-dimensional finite element model for the analysis of transformation hardening processes with temperature dependent optical and thermal material properties. Galantucci and Tricarico [4] proposed two models respectively for stationary and transient processes of laser heat treatment of materials based in the use of the commercial finite element code ANSYS. However, these models lack of a certain physical approach to the real problem of in-process variation of thermal and optical material properties.

Aiming to provide a rather comprehensive solution to the physical problem of laser surface heating of materials using a conventional finite element treatment of geometry, but specially taking into account the very important and sometimes complex physical issues of the laser-matter interaction at the typical intensities of interest, a numerical model, named TEMPLUM, has been developed. This code is able to provide on a time dependent basis, and with spatial resolution only limited by the available computational resources, the evolution of the thermal fields and resulting physical properties of workpieces subject to laser irradiation in surface transformation processes and in any kind of material. TEMPLUM has been successfully tested against experimental results in typical reference configurations, being currently employed for the prediction of thermal fields in a variety of laser surface treatment applications.

2 Code Features

The developed code TEMPLUM [5] is intended to provide the solution to the heat transfer equation in laser surface treatment problems with specific consideration of the particular physical phenomena arising in this kind of processes. Starting from the basis provided by a general purpose finite element code initially intended for the solution of two dimensional heat transfer and electromagnetic problems, TOPAZ [6,7], the mentioned incorporation of particular physical features concerning the problem of laser surface treatments has been undertaken. As a main point, the appropriate treatment of the material workpiece irradiation conditions, with specific consideration of the laser beam spatial energy distribution, the material absorption and attenuation properties along with their variation upon irradiation, and the induced variation of the material thermal properties as a consequence of the laser induced thermal cycles has been envisaged.

In a previous work, Kechemair [3] had considered the possible surface absorptivity variations due to the effects of laser interaction with the workpiece and the definition of a certain average process temperature in order to take into account the resulting variation of the thermal properties of the treated material (35NCD16 steel in that case). However, in the general case the accurate solution of the problem can only be obtained under consideration of a detailed temperature dependence of material properties in the simulation code. On the other hand, very important uncertainties from the practical point of view arise when predicting the real effectiveness of a thermal surface treatment due to an inadequate consideration of the spatial energy distribution of the laser beam (i.e. the real spatial beam profile). In the general case, the energy spatial profile of the irradiating beam differs substantially from any of the currently used limiting cases, and, generally, can only be analytically reconstructed by the superposition of an important number of low order gaussian modes.

In the aim to provide a realistic approach to the general problem of laser treatment of materials in condensed phase (i.e. without consideration of vapour or plasma formation, typical of laser surface treatments without fluid motion), but trying to assess in a proper way both the physical effects of the material thermal and optical properties changes upon laser irradiation as well as the laser irradiation geometry itself (i.e. the full non-linear approach), the TEMPLUM code includes specific modules dealing with the referred problems and allowing to obtain on the numerical side (in principle with no attempt to make any complex interpretation from the material transformations point of view) a high degree of versatility and reliability provided the material constants have been properly specified. On the only basis of the supplied material and process parameters, TEMPLUM is an integrated computational system conceived for the resolution of the heat transfer problem typical of laser-matter irradiation processes with space and time dependent (internal and) boundary sources in 2D or 3D cartesian geometry with specific consideration of the temperature dependence of the material properties i.e. the evolution of the medium transport properties upon development of the laser irradiation. From the mathematical point of view, this corresponds to the resolution of the non-linear heat transfer equation with space and time dependent heat sources:

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (\overline{\overline{\kappa}} \nabla T) + Q(\boldsymbol{r}, t, T) \tag{1}$$

where ρ is the density of the material; Cp is the material heat capacity; T is the material temperature; κ is the material thermal conductivity tensor and Q is the heat source. The boundary conditions needed for the solution of the problem can be specified as:

a) the initial temperature: $T_0 = T(x, y, z, t_0)$
b) the surface convection: $q_C = h \bullet (T-T_E)$
c) the surface radiation: $q_R = \varepsilon \bullet (T^4- T_E^4)$
d) the surface heat flux per area: $q_F = q_F\ (r, t)$

where h is the convective surface heat transfer coefficient, T_E is the absolute temperature and ε is the radiation constant. According to the resolution scheme of the base FEM algorithm, the heat transfer equation is weighted following the standard Galerkin approach as:

$$\int_V w\ \rho C_p \frac{\partial T}{\partial t} dv = \int_V w \nabla \cdot (\overline{\overline{\kappa}} \cdot \nabla \theta) dv + \int_S w Q\, ds \tag{2}$$

where w is an arbitrary variational field satisfying the boundary conditions. The body is approximated geometrically with finite elements, so that the temperature is interpolated as:

$$T = \sum_{i=1}^{i=n} N^i(r)\ T^i = N\ \Theta \quad ; \quad i = 1, 2,.. \tag{3}$$

where T^i are nodal temperatures, N^i are first and second order polynomials in one, two and three dimensions and w, the variational field being interpolated by the same functions:

$$w = \sum_{i=1}^{i=n} N^i(r)\ w^i \quad ; \quad i = 1, 2,.. \tag{4}$$

The variational statement [2] then becomes:

$$\left(\int_V N^i \rho CpN dv\right)\frac{\partial \Theta}{\partial t} =$$
$$= -\int_S N^i q_f\, dS + \int_S N^i h T_E\, dS - \left(\int_S N^i h_c N\, dS\right)\{\Theta\} - \left(\int_V \nabla^T N^i \kappa \nabla N dv\right)\{\Theta\}$$

$$+\int_V N^i q dv \quad (5)$$

or in matrix form

$$[C]\left\{\dot{\Theta}\right\}+[H]\{\Theta\}=\{F\} \quad (6)$$

$$C(\Theta_{n+1}, t_{n+1})\dot{\Theta}_{n+1}+K(\Theta_{n+1}, t_{n+1})\Theta_{n+1}=F_{n+1} \quad (7)$$

and

$$\Theta_{n+1}=\Theta_n+\Delta t\cdot\dot{\Theta}_{n+1} \quad (8)$$

This system is time discretized following the generalised mid-point family of methods with $\alpha=1/2$ (Crank-Nicholson):

$$C(\Theta_{n+\alpha}, t_{n+\alpha})\dot{\Theta}_{n+\alpha}+K(\Theta_{n+\alpha}, t_{n+\alpha})\Theta_{n+\alpha}=F_{n+\alpha} \quad (9)$$

where:

$$\Theta_{n+\alpha}=(1-\alpha)\Theta_n+\alpha\Theta_{n+1} \quad (10)$$

$$\dot{\Theta}_{n+\alpha}=\frac{\Theta_{n+\alpha}-\Theta_n}{\Delta t} \quad (11)$$

$$\Theta_{n+\alpha}=\Theta_n+\alpha\cdot\Delta t \quad (12)$$

The code offers the convergence, stability, accuracy and sensitivity typical of the numerical methods employed [1-4].

Provided that the problem of laser-matter interaction in surface heat treatment applications poses specific difficulties to the resolution of the heat transfer problem in solids, specially in the specification of the heat source (in time dependent of the material state itself) and in what concerns the material non-linear behavior (variable material properties upon temperature evolution), the TEMPLUM system incorporates a set of special routines providing the appropriate treatment of such difficulties, what presents it as a valuable tool for the resolution of the considered problem.

The TEMPLUM code solves the heat transfer equation in two or three dimensional cartesian geometry on the basis of a conventional finite element discretization with rectangular mesh and linear continuous elements. The grid definition and boundary specifications are provided according to the particular problem analyzed. The actual spatial discretization will depend on the process parameters and material properties (determining the code convergence and accuracy), the definition of nodal surface and volume sources to incorporate the different energy deposition and transfer mechanism being a practical need. On the temporal side and provided the specific difficulties posed for the high specific energy derived from the laser matter interaction, an implicit unconditionally stable discretization scheme has been a practical need (Crank-Nicholson; α = 1/2).

For the resolution of the problem, TEMPLUM takes as input parameters the temperature-dependent material optical (i.e. attenuation and absorptivity coefficient) and thermal (i.e. density, heat capacity and conductivity coefficient) properties, the workpiece geometry, the process conditions (laser intensity as heat source) and the configuration parameters of the simulation.

The model provides as output results at any desired time the laser energy input for each node of the defined material mesh, its temperature and heating-cooling rate, the local directional fluxes and the maximum and minimum temperature reached in the mesh. These data unequivocally determine the heat affected zones with expected transformations due to the corresponding thermal cycles.

3 Specific Process Dependent Routines

As a matter of specific interest, the following routines have been implemented into the finite element numerical model for the prediction and analysis of the special problem of laser surface treatments of materials.

3.1 Definition of nodal points, surface and volume elements and boundary conditions

On the one hand, grid nodal points, surface and volume elements have to be defined and, on the other hand, surface elements with boundary conditions due to convection and radiation heat flow and laser beam intensity incidence have to be specified (Fig. 1).

This last characteristic item of the laser processes simulation is discussed in the following sections. The spatial discretization will depend on the piece geometry, process and material type, required accuracy and available computation resources.

The design of the spatial grid for this kind of problem is an example of the experience generally required in this phase, provided such design will affect not only to the result accuracy but also to the calculation economy.

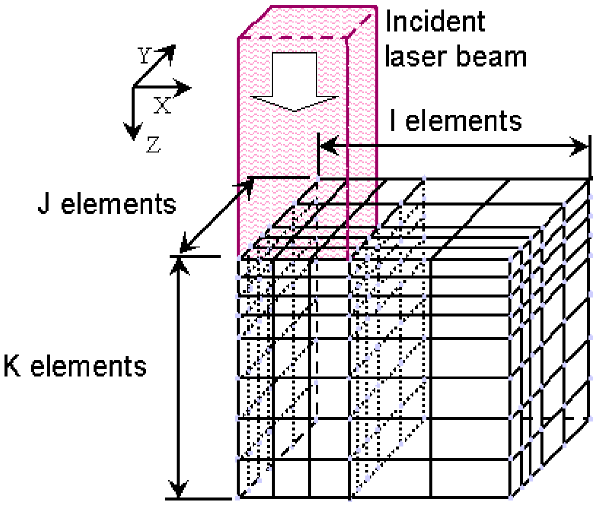

Fig. 1. Definition of nodal surface, volume surface and laser beam incident boundary conditions

3.2 External surface elements with boundary conditions. Concept of absorption factor

The incident laser beam intensity is partially reflected over the material surface depending on the material surface condition and temperature. The relation among the incident, the reflected and the absorbed intensities is given by

$$I = IR + IA = R(T) \bullet I + A(T) \bullet I \quad (13)$$

where R(T) is the reflectivity coefficient and A(T) is the absorptivity coefficient (Fig 2).

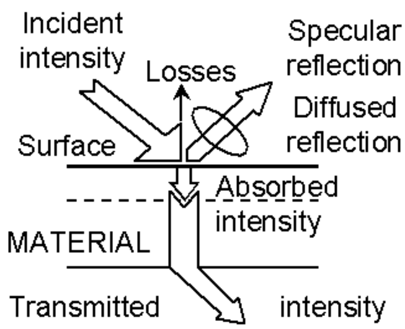

Fig. 2. Intensities diagram during laser-material interaction

3.3 Space and time dependent boundary specification

Boundary conditions due to the laser beam incidence are defined by piecewise linear time-dependent curves (Fig. 3).

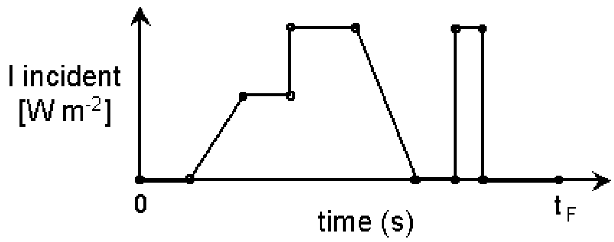

Fig. 3. Piecewise linear temporal function scheme for laser incident intensity

From a general point of view, and depending on the characteristics of the incident laser beam intensity, the processes can be classified into three different categories depending on:

- the piece surface-laser beam relative movement: static (v=0) or dynamic (v≠0) process
- the laser beam intensity distribution: uniform ($I(x,y,z_0) = C$) or non-uniform ($I(x,y,z_0) = f(x,y,z_0)$)
- the laser beam frequency or temporal profile: continuous wave (ν=0) or pulsed (ν≠0) laser

As a result of the combination of these categories, eight cases with different incident intensity function definition can be obtained. Other possible cases need a specific analysis in order to define the surface elements under the incident beam and the number and shape of the incident functions. The figure 4 shows the laser beam incident intensity function for the simulation of a dynamic process with a non-uniform spatial distribution laser beam and with a vibrational component for the beam displacement along the perpendicular axis (OY).

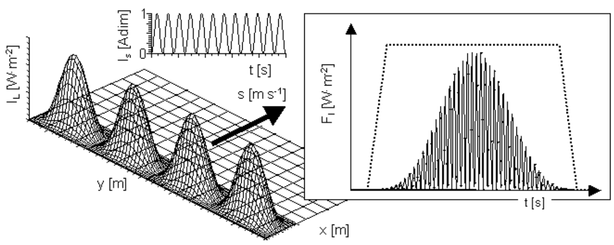

Fig. 4. Spatial and temporal definition of the irradiation conditions for a sample complex case

3.4 Internal surface elements with boundary conditions. Concept of attenuation

In the TEMPLUM input, the incoming intensity is provided as a source load. As an electromagnetic radiation, the laser beam intensity is transmitted inside a material according to the Beer-Lambert law

$$I(z) = I_{z_0} e^{-\alpha z} \quad (14)$$

where I_{z0} is the absorbed intensity at the surface, z is the material depth and α is the attenuation coefficient. This means that, in some cases, not the whole intensity is absorbed in the surface. For the modeling aspects, this implies that can be absorbed intensities in some surface elements not in the grid physical surface. The laser intensity reaching a k surface element with boundary condition due to the laser incidence is given by

$$I_k = I_{z_0} \cdot e^{-\alpha z_k} \tag{15}$$

Then, the intensity fraction that reaches a k surface element and does not reach the following k+1 surface element is given by

$$\Delta I_{a\,k} = e^{-\alpha z_k} - e^{-\alpha z_{k+1}} \tag{16}$$

This intensity fraction is absorbed in the k intermediate volume element (Fig. 5). These coefficients are assigned to all the surface elements under the physical surface elements with boundary condition due to the laser incidence and multiply their corresponding incident intensity function.

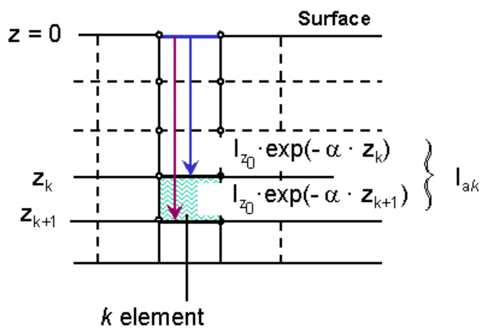

Fig. 5. Transmitted and absorbed intensities scheme

3.5 Temperature dependence of material conducting properties

Temperature-dependent thermal properties (density, heat capacity and thermal conductivity) have already been considered by the FEM base code. These properties can be described by piecewise linear curves and values at intermediate temperatures are obtained by linear interpolation. Additionally and as a major point of relevances, the developed model includes the consideration of the temperature dependent surface absorptivity using the same previous format. However, the model does not explicitly consider the material specific volume changes neither phase transformation enthalpies.

3.6 Specific input/output routines

A set of routines in order to make easy the tridimensional grid generation, the specification of the surface elements with boundary conditions and the definition of the intensity function depending on the process parameters has been developed. This set of routines has been integrated in a computer program in order to prepare the data input file for the computational model.

4 Model Results and Applications

As a preliminary test for checking its performance in a validation test, a comparison between the numerical model results and the bidimensional analytic solution given has been performed. Additionally, the TEMPLUM code has been used for the simulation of several types of problems in the domain of laser surface treatment applications. As a sample of the kind of simulation results that the code can provide, two selected cases will be presented.

4.1 Numerical-Analytical comparison

A comparison between the numerical model results and the bidimensional analytic solution given by Carslaw [8] has been performed for a representative case: the stationary irradiation of an infinite band source determined by $-b < x < b$, $-\infty < y < \infty$ for $z = 0$ (Fig. 6).

$$T(x,z) = \frac{q}{2\pi\kappa} \int_{-b}^{b} e^{v(x-x')/2\chi} K_o\left(\frac{v\sqrt{(x-x')^2+z^2}}{2\chi}\right) dx' \tag{17}$$

where T is the temperature increase in the infinite geometry medium, q is the absorbed intensity, v is the material-source relative speed en the OX axis direction, κ is the material thermal conductivity, χ is the material thermal diffusivity and K_0 is the modified Bessel function. For a semi-infinite solid ($z > 0$), the temperature increase is multiplied by 2.

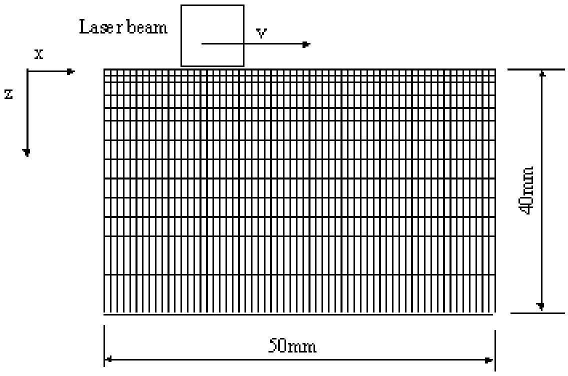

Fig. 6. Typical 2D grid used by the model

Due to the analytic model limitations, temperature-independent material properties are considered. The complete input data and process parameters are shown in Table 1.

Table 1. Process parameters for the 2D analytical-numerical model results comparison

Material	Mild steel
Mesh geometry	Rectangular
Mesh dimension	50 x 40 mm
Density	7860 kg m^{-3}
Heat capacity	600 J kg^{-1} K^{-1}
Thermal conductivity	32 W m^{-1} K^{-1}
Material absorptivity	$\approx \infty$ m^{-1}
Surface absortance	1
Initial temperature, T_o	27°C
Intensity distribution	Uniform
Beam dimensions	10 mm
Beam intensity	10^7 W m^{-2}
Material-laser relative speed	10 mm s^{-1}
Final time	4 s

For the numerical model simulation the grid dimensions are large enough (thickness=40mm and length=50mm) to be considered equivalent to the semi-infinite geometry of the analytic solution and to reach the stationary process (t>3s). The figures 7 and 8 show both results.

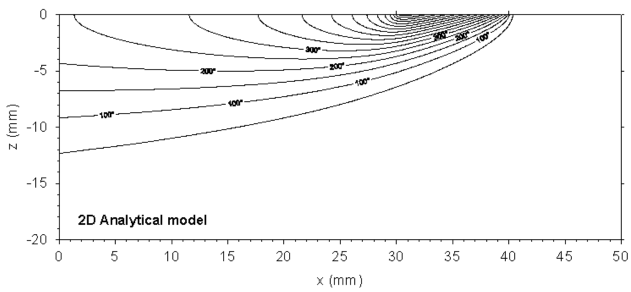

Fig. 7. Temperature increase prediction for a laser heating treatment of mild steel obtained with the analytic 2D model.

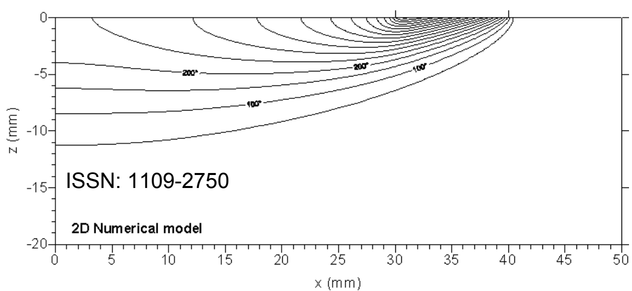

Fig. 8. Temperature increase prediction for a laser heating treatment of mild steel obtained with the numerical 2D model

The figure 9 compares the temperature increase obtained in points belonging to the surface perpendicular axis that cross the maximum-temperature node. The maximum difference between these results is not bigger than 0.5% (2°).

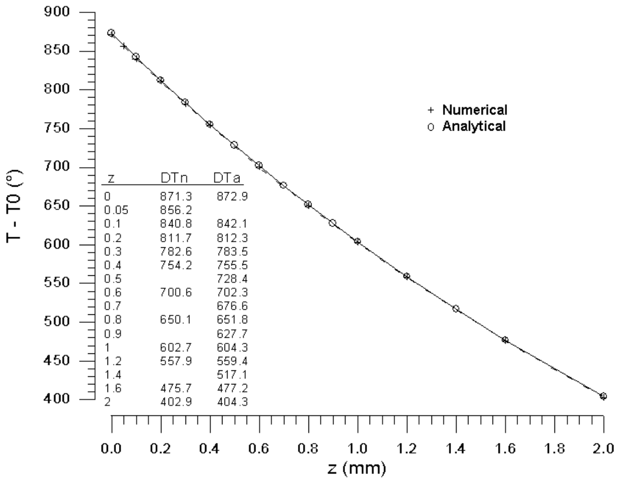

Fig. 9. Analytical-numerical results comparison

These differences are similar to other results from comparisons between analytical and numerical methods of solving transient heal conduction problems [9].

4.2 Laser surface treatment of F1140 carbon steel with a CO_2 laser beam

In this sample case, the standard possibilities of the code as a prediction tool for the transformation hardening of steels (the primary and most conventional application of the code since the first studies) will be presented [9]. For the development of this kind of application, the laser beam, coming from an optical resonator delivering a continuous average power in the range 1300-1700 W, incided on a 100x20x5 mm^3 material workpiece of the referred steel with temperature dependence material properties (Fig. 10-12) and irradiation parameters given in Table 2.

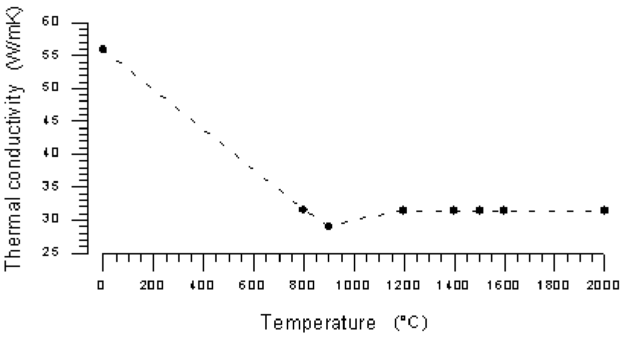

Fig. 10. Temperature dependence of F1140 steel conductivity

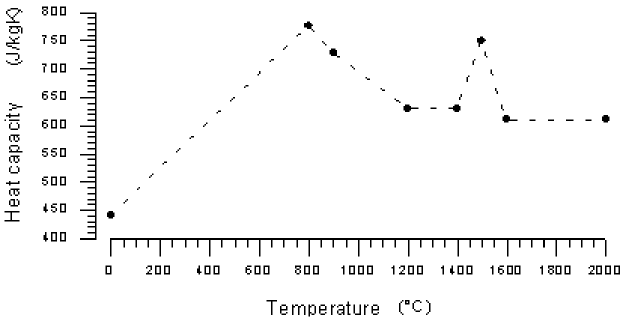

Fig. 11. Temperature dependence of F1140 steel heat capacity

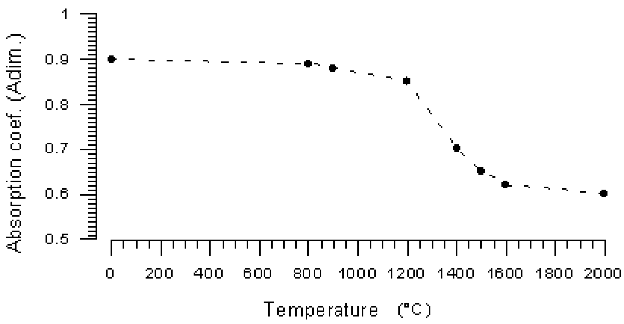

Fig. 12. Temperature dependence of F1140 steel absorption coefficient

Table 2. Irradiation parameters considered in the laser surface treatment of F1140 steel with a CO_2 laser beam

Irradiation parameters (unit)	*Values*
Irradiation power (W)	1300±2%
Irradiation wavelength (μm)	10.6
Beam characteristic diameter (mm)	4
Beam divergence (mrad)	≤ 1.5
Beam average intensity (Wcm^{-2})	≈10^4
Spatial beam distribution mode	Gaussian TEM_{01*}

The considered processes aim the transformation of the microstructure of the workpiece surface and, consequently, the derived mechanical properties. According to this, a fundamental element for the evaluation of the results of the code will be the analysis of the zones in which the mechanical properties have suffered a change as a consequence of the temperature increase induced by the laser beam. On the basis of this procedure, an indirect (while rather accurate) evaluation of the thermal history of the points of the workpiece clearly indicating the maximum extent of the thermal fields respect to the critical temperatures for steel transformations was used. For the prediction in the numerical simulations of the zones really suffering the metallurgical transformations the influence of the heating-cooling speed on the transformation points was considered. As a sample of the results provided by the model, in figure 13 and 14, the thermal cycle and heating–cooling rates for points of the test piece in the symmetry plane of a 1300 W laser beam are respectively given, and, in figure 15, the final stationary isotherms of the test piece are shown with an specific indication of the zones for which the transformation heat of the steel is predicted, what will be specially suitable for comparison to experimental results.

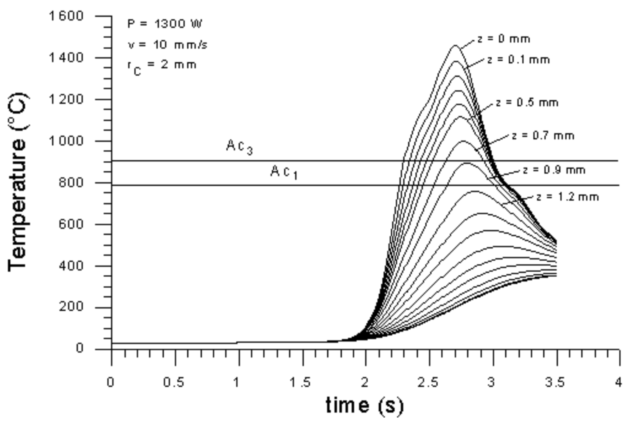

Fig. 13. Material thermal cycle prediction at different depth nodes obtained for a steel plate upon a 1300 W TEM $_{01*}$ CO_2 laser irradiation

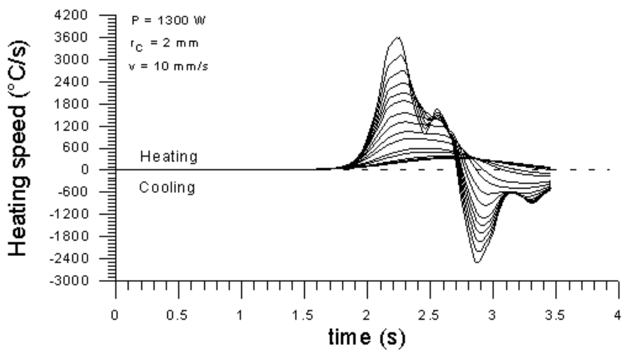

Fig. 14. Heating-cooling rates prediction at different depth nodes obtained for a steel plate upon a 1300 W TEM $_{01*}$ CO_2 laser beam

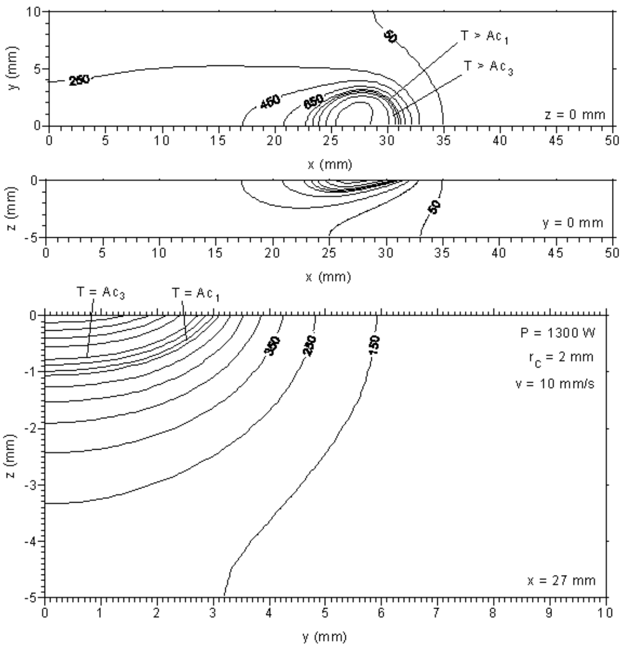

Fig. 15. Prediction of final stationary spatial distribution of temperatures field for a test piece treated with 1300 W TEM_{01*} CO_2 laser beam

In Fig. 16, a metallographic cut is shown of the workpiece to be compared with the corresponding predicted transformation map.

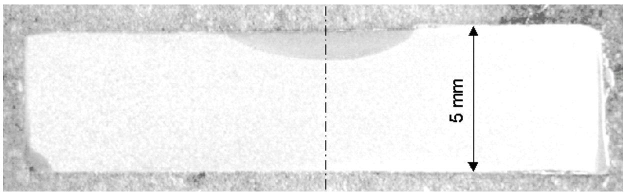

Fig. 16. Metallographic cross section of a laser hardened F1140 steel sample irradiated with a 1300 W TEM_{01*} CO_2 laser beam

The agreement between theory and experiment is remarkably good, what can be quantitatively assessed through the microhardness profile (Vickers Test) shown in Fig. 17, where the completely transformed zone and the transition zone are clearly defined.

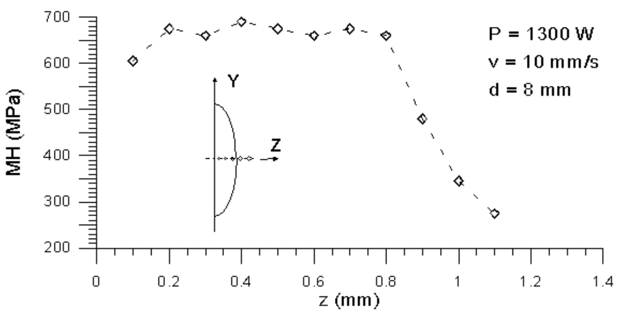

Fig. 17. Microhardness profile of a laser hardened F1140 steel plate irradiated with a 1300 W TEM_{01*} CO_2 laser beam

The comparison between the experimental and numerically predicted results in this case is shown in Table 3 and is to be considered as certainly good provided the uncertainties assumed in the material and interaction physical properties.

Table 3. Comparison between predicted and experimental results for transformation hardening of F1140 steel with 1300 W TEM_{01*} CO_2 laser beam

Parameter	*Measured*	*Predicted*	*Relative Error*
Tempered seam width y_1 (mm)	6.50±0.01	6,20	-4.62%
Tempered seam depth z_1 (mm)	0.98±0.01	1,10	+12.24%
Partial tempering depth z_3 (mm)	0.80±0.01	0.85	+6.25%

4.3 Laser surface treatment of B-270 optical glass with a conformed CO2 laser beam

In order to show from a theoretical point of view the possible differences between the thermal effects induced in materials by uniform and non-uniform irradiation patterns, and as a test for the simulation capabilities of the described model, the simulation with the aid of TEMPLUM of a real experimental procedure in the domain of optical glass polishing by laser has been performed.

Concretely, a comparative analysis between the thermal effects induced in optical glass by both uniform and regularly peaked laser intensity distributions aiming to reproduce the intensity patterns resulting from optical beam conformation by faceted mirrors [10, 11] has been performed.

For this comparison, the material considered has been a 5 mm thick infinite slab of B-270 optical glass with material and optical properties given in Table 4 preheated to 550ºC.

Table 4. Properties of B-270 Glass

Property (units)	*Value*
Absorption coefficient (m^{-1})	7.10 10^4 (λ=10,6 μm)
Density ($kg.m^{-3}$)	2.5 10^3
Specific heat ($J.kg^{-1}.K^{-1}$)	10^3
Thermal conductivity ($W.m^{-1}.K^{-1}$)	1.047+0.001489.T (T<900ºC) 2.387 (T>900ºC)

The considered irradiation patterns have been a uniform beam power P_0=58 W extended to the square $|x|<l/2$, $|y|<l/2$ and, as an opposite case, a regularly peaked profile responding to the functional distribution:

$$I(x,y)=\begin{cases} I_0 \operatorname{sen}^8\left(\frac{2\pi}{d}x\right)\operatorname{sen}^8\left(\frac{2\pi}{d}y\right) \text{for} |x| \le l/2; |y| \le l/2 \\ 0 \ \text{ for} |x| > l/2; |y| > l/2 \end{cases} \quad (18)$$

(with d = 1.2 mm and l = 8.4 mm) extended over the same square, so that, as it can be simply verified, the average intensity of the latter is exactly coincident with the value P_0 (corresponding to the uniform beam). In Fig. 18 the resulting thermal fields distributions at the irradiated surface are shown for a characteristic irradiation time (1.5 seconds in both cases) for the two cases under comparison.

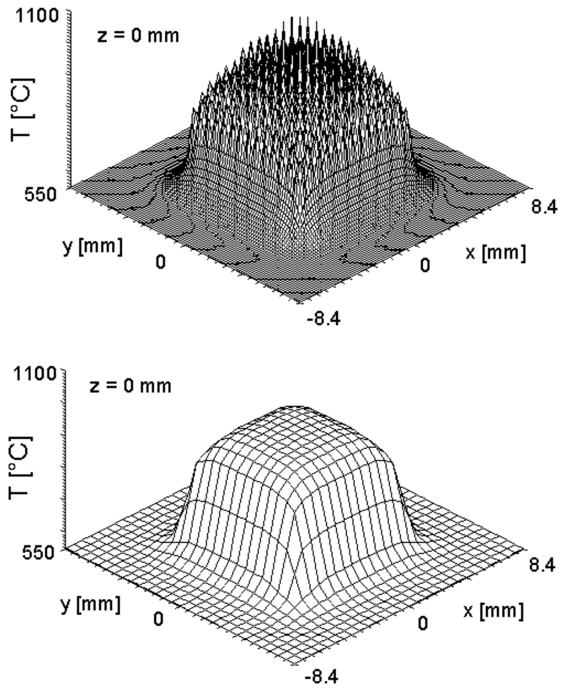

Fig. 18. Temperature field predictions in B-270 glass test piece irradiated with regularly peaked intensity distribution beam (top) and uniform intensity pattern distribution (bottom)

From a simple visual inspection of both figures, significant differences can be observed between the thermal conditions reached in either case. Not only the maximum temperature values obtained in the piece are significantly different (900ºC in the uniform irradiation case versus 1060ºC in the case of the regularly peaked intensity profile), but also the thermal gradients induced in the material are significantly different (both along the depth and laterally for a given depth) from case to case. From a computational point of view, the analyzed case provides a valuable sample of the capabilities of the model for the simulation of laser material treatments. Not only for surface treatment purposes in metals with extremely high attenuation coefficient and reasonably good thermal conductivity, but also in materials with low conductivity in which the radiation has a finite penetration (as the optical glass considered). In these zones the thermal gradients can be extremely high and can cause important problems to the numerical discretization schemes. The use of TEMPLUM with well selected discretization parameters has proved to be a extremely consistent and robust tool for the simulation of laser materials treatment in condensed phase even in cases where other similar simulation tools have shown great difficulties. As recognized in the previous section, from a physical point of view, the problem of laser polishing of optical glass with optically conformed laser beams, although not directly related to applications of laser surface treatment of metals, has to be considered as a decisive kind of experiments able to pose the most difficult problems to a numerical simulation tool as the described one in order to provide accurate results. In fact, the initial prospects of the analysis of such kind of treatments made by the authors came into play as a consequence of the difficulty to predict the maximum temperature reached by the glass found by experimenters in routine application of the technique. The application of TEMPLUM to the resolution of the problem was in fact quite direct with the aid of the pre-processing and on-line routines of the code (specially suited for the kind of problems considered) and provided the desired results in a way directly amenable to comparison with experimental results. In Fig. 19 a surface thermal map is presented of the test piece treated in which the melting isotherm is shown to enclose the melt zones of the glass that can be directly correlated to the zones actually molten in the corresponding experiment.

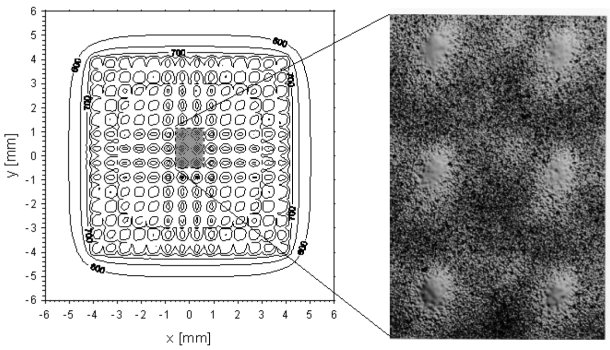

Fig. 19. Surface thermal map of B-270 glass showing zones of predicted melting (left) and photograph showing molten zones in B-270 glass after laser irradiation (right)

5 Conclusions

In view of the presented results and the specific properties of convergence, stability and accuracy directly evaluated in previous work [5], the TEMPLUM code has to be considered as a valuable numerical simulation tool comparable to the most advanced codes developed for the prediction of the dynamical behavior of thermal fields in matter following external heating. Additionally, provided the set of specific routines added to the numerical basis of the code in order to handle the particular features of laser material treatment applications in condensed phase, including the allowance for temperature and process dependent optical and thermal material properties and its inherent ability to take into account special process-oriented boundary conditions, the TEMPLUM code has to be considered as a really useful tool for the predictive assessment of laser surface treatment applications in a broad variety of processes of industrial interest. In these special cases, the tool cannot be compared to other alternatives (that not consider these conditions) but to experimental results. Some opportunities and new developments in the future of this work include the analysis of the laser heat treatment in extended surfaces [14], the prediction of the material hardness after the heat treatment [15] and the application of these results in hybrid fuzzy logic control of laser surface treatments [16].

References:

[1] Mazumder, J. and Steen, W.M. *Heat Transfer Model for CW Laser Material Processing*, Applied Physics, 51, 1980, pp. 941.

[2] Fritsch, H. U. and Bergmann, H.W. Influence of the Carbon Diffusion During Laser Transformation Hardening. *Numerical Simulation and Experimental Verification*, Diehl GmbH and Co, Röthenbach, Germany, 1982.

[3] Kechemair, D. *Instrumentation et Optimization de la Trempe Superficielle des Aciers par Laser CO2 Continu*, Thèse Doctorale. Université de Paris-Sud, 1989.

[4] Galantucci, L. and Tricarico, L. Transient Numerical Analysis of Laser Heat Treatment using FEM, *Proc. LANE'94*, Vol. I. M. Geiger y F. Volltersen (eds), Meisenbach Bamberg, 1994.

[5] García-Beltrán, A. *Desarrollo y Validación de un Modelo Computacional para la Predicción y Caracterización de Procesos de Tratamiento Térmico Superficial de Materiales con Láser*, PhD Thesis, Universidad Politécnica de Madrid, 1996.

[6] Shapiro, A. B. and Edwards, A. L. TOPAZ2D, *Heat Transfer Code Users Manual and Thermal Property Data Base*, Report UCRL-ID-104558 (rev. 1), University of California, Lawrence Livermore National Laboratory, 1990.

[7] Shapiro, A. B. *TOPAZ3D - A Three Dimensional Finite Element Heat Transfer Code*, Report UCID-20484, University of California, Lawrence Livermore National Laboratory, 1985.

[8] Carslaw, H. S. and Jaeger, J. C. *Conduction of Heat in Solids*, Oxford University Press, 1959

[9] Riyad, M. and Abdelkader, H. *Comparison between the Analytical and Numerical Methods of Solving One-Dimensional Transient Heat Conduction Problems*, Proc. of the 4th WSEAS Int. Conf. on Heat Transfer, Thermal Engineering and Environment, Elounda, Greece, 2006, pp. 380-384.

[10] García-Beltrán, A. and Ocaña, J. L. Modelo Numérico Tridimensional para la Simulación de Procesos de Tratamiento Superficial de Materiales con Láser, *Rev. Metal. Madrid*, 35 (2), 1999, pp. 75-83.

[11] Laguarta, F., Lupón, N. and Armengol, J. Optical Glass Polishing by Controlled Laser Surface Heat Treatment, *Applied Optics*, 33, 1994, pp. 6508-6513.

[12] Ocaña, J. L. et al. Analysis of the Effect of Optically Induced Local Non-Uniformities in Laser Surface Treatment Applications, *Proc. of 1996 Conference on Lasers and Electro-Optics Europe (CLEO/EQEC)*, 1996.

[13] Ocaña, J. L. et al. Laser Heat Treatments Driven by Integrated Beams: the Role of Irradiation Non-Uniformities, *Applied Optics* 38 (21), 1999, pp. 4570-4576.

[14] García-Beltrán, A. et al. Análisis de la influencia del factor de solapamiento en el tratamiento térmico de superficies extensas de aceros por láser, *Rev. Metal. Madrid*, 43 (4) 2007, pp. 284-293.

[15] Jonczyk, S. et al. *Computer Hardness Prediction of Steel after Quenching, with a Proatable Quench Tester*, Proc. of the 4th WSEAS Int. Conf. on Heat Transfer, Thermal Engineering and Environment, Elounda, Greece, 2006, pp. 175-179.

[16] Pérez, J. A. et al. Hybrid Fuzzy Logic Control of Laser Surface Heat Treatments, *Applied Surface Science*, 254 (2007), pp 879-883.