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Numerical Model for Transient Analysis of Multilayer Thin Films Irradiated by a Moving Laser Source

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Abstract: A two-dimensional transient analysis of the conjugate optical-thermal fields induced in a multilayer thin film structure on a glass substrate by a moving Gaussian laser source is carried out numerically. The workpiece is considered semi-infinite along the motion direction and its optical and thermophysical properties are assumed temperature dependent. The COMSOL Multiphysics 3.3 code has been used to solve the combined thermal and electromagnetic problem. The optical field is considered locally one dimensional and Maxwell equations are solved in order to evaluate the absorption in thin film. Results, in terms of transient temperature profiles and fields, are presented for different Peclet numbers and starting point of the heat source with respect to the workpiece boundary along the motion direction.

Keywords: Combined Heat Conduction and Radiation, Laser Source, Moving Sources, Thin Films, Manufacturing.

1. Introduction

High energy density sources are widely used in material manufacturing and processing. This is due to the existence of new materials and to the use of innovative processes employing laser and electron beam, such as welding, cutting, heat treating of metals and manufacturing of electronic components. As laser applications become more demanding, a thorough understanding of the thermal coupled conductive-radiative phenomena involved is required. So in the last decades many research efforts were dedicated to the development of analytical and numerical models in order to predict the thermal fields induced by stationary or moving heat sources (Shah et al. [1]; Tanasawa and Lior [2]).

The interaction between a laser source and a multilayer thin films have been widely investigated because of its extensive application in many fields. Depending on the wavelength of the heating laser pulse, the optical properties of materials in thin films are generally temperature dependent. These induce a thermally optical nonlinearity [3].

Tamura et al. [4] carried out one of the first studies on the one-dimensional coupled problem for a single and multilayer thin film on a glass substrate. Grigoropoulos et al. [5] solved the coupled optical-thermal problem, and the evaluation of energy absorption was obtained by a thin optic model. Chen and Tien [6] employed a similar model to examine the effects of temperature-dependent optical characteristics. The conjugate optical and thermal fields in a multilayer thin film irradiated by a pulsed laser beam was analyzed in [7]. Optical and thermal properties were assumed temperature dependent. Bianco and Manca [8] extended the analysis presented in [7] to a two-dimensional problem. For a multithin film structure, irradiated by a circular gaussian laser beam, a numerical model was proposed by Nakano et al. [9]. They considered an absorbed laser power density with an exponential decay for each layer in the thermal model. McGahan and Cole [10] extended the theory presented in the previous paper to include anisotropic thermal properties. Bianco et al. [11] analyzed numerically the coupled optical-themal field in a thin film on a glass substrate irradiated by a moving continuous laser source in quasi-steady state conditions. The heat transfer and the deformation in an acrylonitrile-butadiene-styrene (ABS) plastic by using Nd:YAG pulse laser irradiation was analyzed in [12] both numerically and experimentally.

In this paper the two-dimensional conjugate optical-thermal model in a multilayer thin film irradiated by a moving laser source is numerically solved. The multilayer thin film (composed by a a-Si layer and a TCO one) is deposed on a glass substrate and it is irradiated by a Gaussian moving laser beam. Since the optical and thermal fields are strictly linked, this problem is solved by means of COMSOL Multiphysics 3.3. The model extends to a semi-infinite workpiece the analysis given in [12].

Results are evaluated for a countinous moving laser source and they are presented in terms of temperature profiles and fields.

2. Mathematical Description

The investigated object is composed by an amorphous silicon layer thin film deposited over a TCO layer and a glass substrate, figure 1. A Nd-YAG source is chosen and its wavelength is 1064 nm. Laser beam is continous and irradiates the a-Si layer surface. Moreover, a Gaussian distribution moving at constant velocities is considered. The solid dimension along the motion direction is assumed to be as semi-infinite (L_x = 5 mm), while finite thicknesses for TCO (s_t) and a-Si layers (s_s) are considered. Thermal and optical properties are assumed as

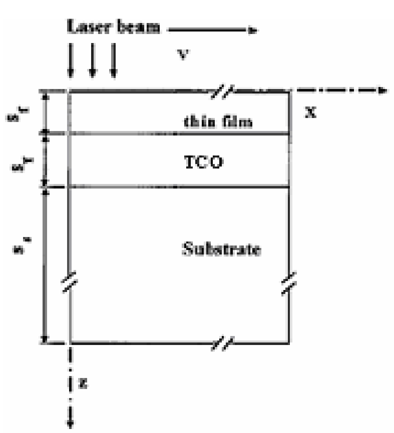


Figure 1: Sketch of the thin film and the TCO layer on glass substrate.

functions of temperature and the materials are considered isotropic. Thermal radiation is absorbed within the whole thin film thickness and absorption mechanism is modelled as a thermal generation as shown in the heat conduction equation. Radiative and convective heat losses from the surfaces toward the ambient (a-Si interface) are neglected and the thin film can be treated as a semitransparent material, due to its small thickness.

In a coordinate system fixed to the heat source, according to the theory of moving heat source [14], a mathematical statement of the thermal conductive problem is:

$$\frac{\partial}{\partial x}\left(k_i(T)\frac{\partial T_i}{\partial x}\right)+\frac{\partial}{\partial z}\left(k_i(T)\frac{\partial T_i}{\partial z}\right)+ + \dot{u}'''(T_i,x,z)=\rho c\left(\frac{\partial T_i}{\partial \theta}-v\frac{\partial T_i}{\partial x}\right) \quad (1)$$

with i = f, t or s and for $0 \le x < L_x$, $0 \le z \le s_f + s_t + s_s$, θ>0; with s_f the thin film thickness, s_t the TCO thickness and s_s the substrate thickness.

The boundary and initial conditions are reported in the following relations:

$$T_i(x,z,0)=T_{in} \quad (2a)$$

with i=f, t or s, for $0 \le x < L_x$, $0 \le z \le s_f + s_t + s_s$, θ>0

$$-k_f\frac{\partial T_f(x,0,\theta)}{\partial z}=0 \quad (2b)$$

for $0 \le x < L_x$, θ>0

$$-k_s\frac{\partial T_s(x,s_f+s_t+s_s,\theta)}{\partial z}=0 \quad (2c)$$

for $0 \le x < L_x$, θ>0

$$k_f\frac{\partial T_f(x,s_f,\theta)}{\partial z}=k_t\frac{\partial T_t(x,s_f,\theta)}{\partial z} \quad (2d)$$

for $0 \le x < L_x$, θ>0

$$k_t\frac{\partial T_t(x,s_f+s_t,\theta)}{\partial z}=k_s\frac{\partial T_s(x,s_f+s_t,\theta)}{\partial z} \quad (2e)$$

for $0 \le x < L_x$, θ>0

$$-k_i\frac{\partial T_i(0,z,\theta)}{\partial x}=0 \quad (2f)$$

with i=f, t or s, for $0 \le z \le s_f + s_t + s_s$, θ>0

$$T_i(L_x,z,\theta)=T_{in} \quad (2g)$$

with i=f, t or s, for $0 \le z \le s_f + s_t + s_s$, θ>0

The generation term $\dot{u}'''(T_i, x, z)$ is assumed as depending on optical material properties and is related to the Poynting vector S, by means of equation (4). The S evaluation is made by means of Maxwell equations and following the COMSOL indications:

$$S = \frac{n_a}{2\mu c'}|E_a|^2 \quad (3)$$

and the absorbed energy for unit volume:

$$\dot{u}'''(T_f, x, z) = -\frac{\partial S(x,z)}{\partial z} \quad (4)$$

The laser source irradiation is given by:

$$I(x) = I_0 \exp\left[-\left(\frac{x^2}{r_g^2}\right)\right] \quad (5)$$

The term r_g is the radius of the Gaussian laser beam. One of the typical parameters that describe the investigated problem is the Peclet number. It represents the ratio between the convective and diffusive terms along the motion direction $Pe = (v\, r_g)/(2\, \alpha)$.

The two dimensional conductive field and the one dimensional local optical field for absorbing thin films are solved by means of the COMSOL Multiphysics 3.3 code.

3. Numerical Model

The investigation is carried out for a solid composed by an amorphous silicon film layer with a thickness equal to 0.5 μm while the thickness of TCO layer and glass substrate is 0.6 μm and 500 μm, respectively. Thermophysical and optical properties of the employed materials are reported in table 1 and table 2.

The laser power is set to 0.30 W and a beam radius of 25 μm is chosen. The irradiation distribution is Gaussian and the heat source moves along *x* axis from $x_0 = m^* r_g$ with m equal to 0, 1, 2 and 5. Different constant velocities are considered in order to correspond to Peclet numbers equal to 1.0, 2.0, 3.0, 4.0 and 5.0.

Four different grid distributions have been tested to ensure that the calculated results are grid independent. The following configuration has been chosen: the film layer has been subdivided into 150 nodes while the number of nodes in the TCO layer is 100 and 600 for glass substrate. The number of nodes in the axial direction is 200. The grid mesh is structured. The maximum temperature differences of the fields are less than 0.1 precent by doubling the mesh nodes.

Table 1: Thermophysical properties of the employed materials

	k [W/mK]	ρc_p [J/m^{3}K]
glass	1.4	1200
TCO	39.6–2.09 x 10^{-2} (T-273.15)+4.62 x 10^{-6} (T-273.15)^2	371 +0.217 (T-273.15)] 6640
a-Si	1.3 x 10^{-9}(T-900)^3 +1.3 x 10^{-7}(T-900)^2 +10^{-4}(T-900)+1.0	[(171/T)/685+ 952] 2330

Table 2: Refractive index of employed materials for λ = 1064 nm.

	$\bar{n} = n - ik_{est}\ (\lambda = 1064nm)$
glass	1.46-i 0.0
TCO	1.95 – 0.002
a-Si	3.8 – i [0.0443 + 6.297 x 10^{-5} (T-273.15]

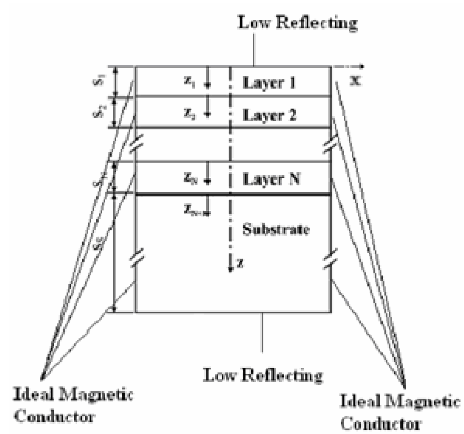


Figure 2: Thin film, TCO and glass substrate optical model.

In order to analyze the coupled optical-thermal fields an electromagnetic and a thermal model have been developed. This combined problem has been studied by means of Comsol Multyphisics 3.3. It has been necessary to adopt the *"In-Plane Waves Application Mode"* and an armonic propagation analysis of *TE* waves has been chosen. The laser beam is orthogonal to the target and the radiative field related to the absorprtion-reflection-transmission process in the thin film structure is locally one-dimensional and so, suitable boundary conditions in the electromagnetic model have been applied, as shown in figure 2.

The two-dimensional heat conduction equation are solved by using the *"Heat Transfer Module"* and a *"Transient analysis"* in *"General Heat Transfer"* window for the thermal model.

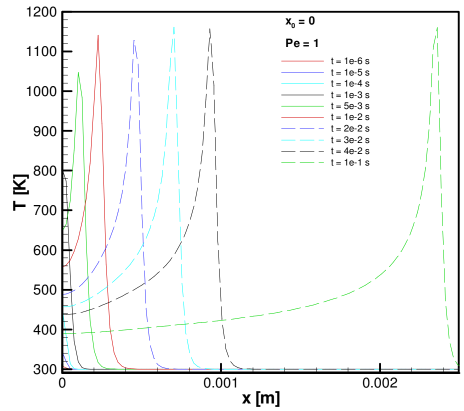
4. Results and Discussion

Results related to an amorphous silicon thin film deposited on a TCO layer and a glass substrate, in terms of temperature profiles and fields, are presented in the following.

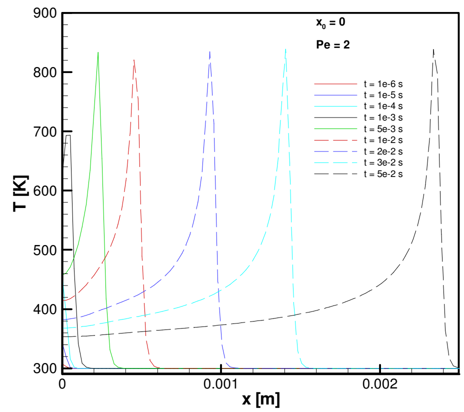
Figure 3 reports temperature profiles along x-direction for different Peclet numbers and $x_0 = 0$. They have been evaluated at the film surface (z=0.0 m). It is observed in figure 3.a that the laser spot starts to warm up the zones near the origin. At t = 1×10^{-3} s the temperature maximum is attained far from the origin and the maximum intensity of irradiation has moved to x = 2.36×10^{-5} m. At t = 5×10^{-3} s a maximum temperature equal to 1040 K is reached and it is localized far from origin. The highest temperature (1163 K) is detected at t = 1×10^{-2} s. Quasi-steady state condition has not been detected. Furthermore, temperature profiles change increasing the time because the heat affected zone grows while the temperature peaks keep constant. For increasing Peclet numbers (fig. 3.b and fig. 3.c), it's evident that the maximum temperatures are attained in correspondance with larger times. Furthermore, temperature peaks decreases as Peclet number increases. For each configuration temperature values augment near the origin then they tend to decrease because the absorbed thermal energy has diffused in the solid. Asymptotic temperature values raises as Pe numbers decrease.

Figure 4 describes the develop of the transient temperature profiles along x-axis for different starting positions of the laser spot and Pe = 2.0. In particular, it has been considered a distance from the origin, x_0, equal to 1 (fig. 4.a), 2 (fig. 4.b) and 5 r_g(fig. 4.c). It is observed that the temperature peaks detected are constant, considering the three cases. Some differences are noticed in the zones near the origin. At the beginning of the warm up the heat affected zone grows as increasing x_0. It's remarkable to point out that the zones localized near the origin are as much colder as x_0 augments for t > 1×10^{-2} s.

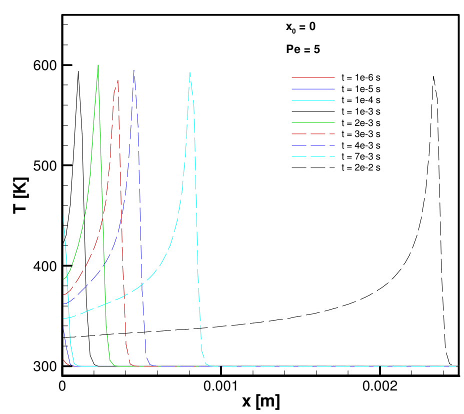
Figure 5 exhibits a comparison among the temperature profiles along x-axis for different



(a)



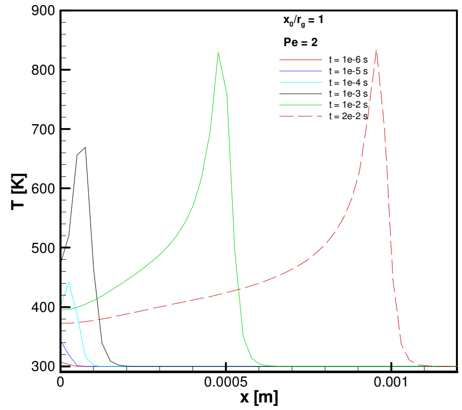
(b)



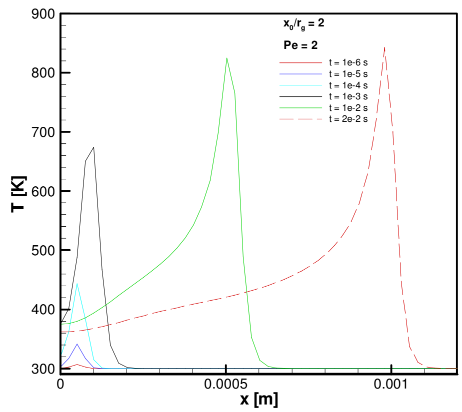
(c)

Figure 3: Temperature profiles at surface for different Peclet numbers equal to 1.0 (a), 2.0 (b) and 5.0 (c) and $x_0 = 0$.

values of Peclet numbers and x_0 = 0 in quasi-steady state condition. It is observed that the smaller is the Peclet number the larger is the attained temperature.Furthermore, the zones not



(a)



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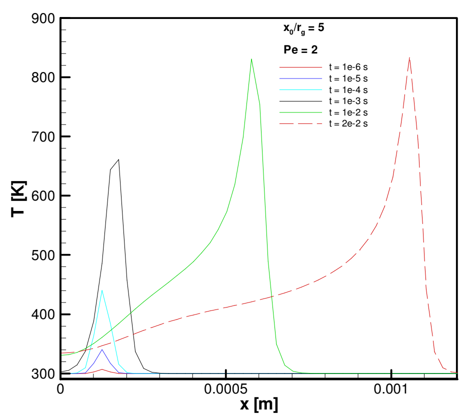


(c)

Figure 4: Temperature profiles for different source starting positions, $x_0 = m*r_g$ with m = 1 (a), 2 (b), 5 (c) and Pe = 2.0.

irradiated by the spot show more evident diffusion phenomena. In correspondence with origin, temperature reaches higher value as Peclet numbers decrease.

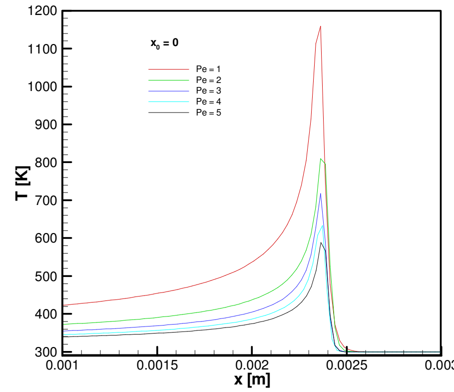


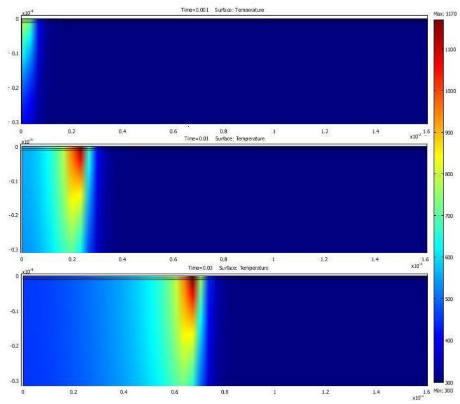
Figure 5: Temperature profile along x-direction for Peclet numbers equal to 1.0, 2.0, 3.0, 4.0 and 5.0 and $x_0 = 0$.

In Figure 6 temperature fields for $x_0 = 0$ and Pe = 1.0 and 5.0 are reported at three different times ($1x10^{-3}$ s, $1x10^{-2}$ s and $3x10^{-2}$ s). For the lowest considered Peclet number (fig. 6.a), it is observed the development of the thermal affected zone inside the semi-infinite solid. At the first considered time, the thin film is almost isotherm whereas the glass substrate presents some temperature gradients. In this zone the heating is due only at the conductive heat transfer because the glass is assumed as a perfect non-absorbent media. In the next time, the thin film achieves maximum temperatures and the heat affected zone grows close to the highest value of the heat source whereas the zones close to the origin present lower temperature. At the last considered time the heat affected zone is slightly wider. It's interesting to point out the effects of diffusion along the motion direction. In Figure 6.b, for Pe equal to 5.0, the temperature field shows lower temperature values, greater temperature gradients along x-axis and a reduced penetration length and less diffusive effects.

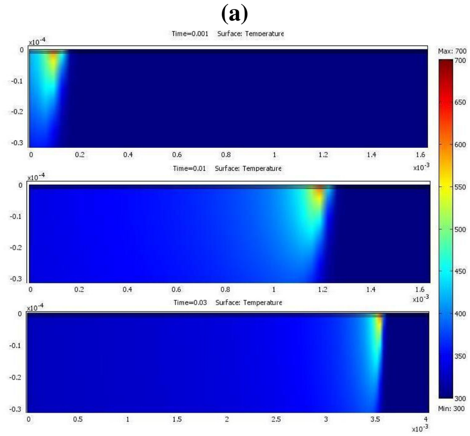
In Figure 7, temperature fields are presented for $x_0 = 5*r_g$ and Peclet numbers equal to 1.0 and 5.0, for the same times as the previous figure. Comparing these fields with the previous ones, the most evident difference is at first considered times, where temperatures are lower close to the origin and the heat affected zone is wider.

5. Conclusions

A combined optical and thermal fields induced in a multilayer thin film on a glass

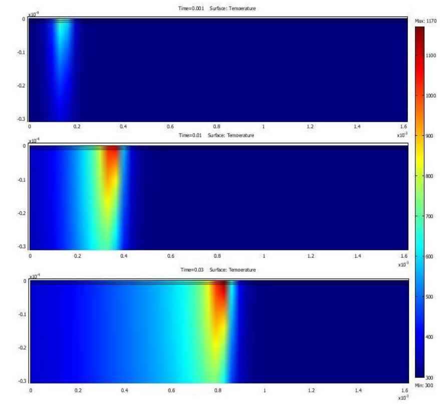


(a)

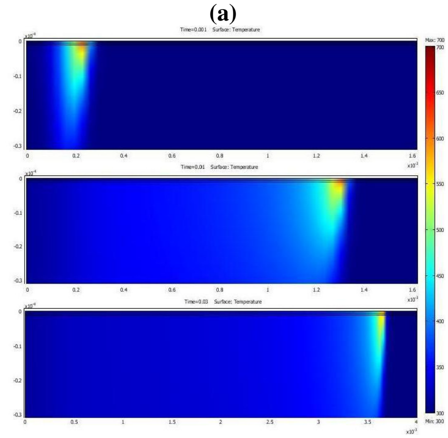


(b)

Figure 6: Temperature fields for Pe = 1.0 (a) and 5.0 (b) and $x_0 = 0$ at $t = 1x10^{-3}$ s, $t = 1x10^{-2}$ s and $t = 3x10^{-3}$ s



(a)



(b)

Figure 7: Temperature fields for Pe = 1.0 (a) and 5.0 (b) and $x_0 = 5\ r_g$ at $t = 1x10^{-3}$ s, $t = 1x10^{-2}$ s and $t = 3x10^{-3}$ s.

substrate by a moving laser source was investigated in this paper. The transient two-dimensional analysis was carried out numerically, by means of the COMSOL Multiphysics 3.3 code, for a semi-infinite workpiece along the heat source motion direction. Temperature profiles and fields showed that the maximum temperature value reached within the structure at the quasi-steady state condition decrease at increasing Peclet number. The transient analysis showed that the time at which the maximum temperature is attained increased with the Peclet number. Results for different starting point of the heat source showed a strong influence of this parameter at the beginning of the warm up, whereas its effect vanished as time increased.

6. Nomenclature

c = specific heat, J kg^{-1} K^{-1}
c' = speed of light, m s^{-1}
E = electric field, N C^{-1}
k = thermal conductivity, W m^{-1} K^{-1}
k_{est} = extinction coefficient
n = real part of refractive index
$\bar{n}$ = complex refractive index
Pe = Peclet number, $(v\ r_g)/(2\ \alpha)$
r = radius, m
S = Poynting vector, W m^{-2}
T = temperature, K
t = time, s
$\dot{u}'''$ = generation function, W m^{-3}
x,z = spatial coordinate

6.1 Greek symbols

λ = wavelength, m
μ = magnetic permeability, N s^2 C^{-2}
ρ =density, kg m^{-3}

6.2 Subscripts

a = air
f = film
g = Gaussian
in = initial
l = length
0 = starting source position
p = peak
s = substrate
t = TCO layer

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