Transient Conjugate Optical-thermal Fields in Thin Films Irradiated by Moving Sources: a Comparison between Back and Front Treatment

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Abstract: A two dimensional instationary 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 in order to compare back and front laser treatment processes. The workpiece is considered semi-infinite along the motion direction. Thermal and optical non-linearities are induced during transient heating, since the response of weakly absorbing thin films depends on temperature. The heat source can either directly impinge the film surface (front laser treatment), or the glass substrate (back laser treatment). COMSOL Multiphysics 3.4 code has been adopted to solve the combined thermal and electromagnetic problem in order to compare the two processes. The optical field is considered locally one dimensional and Maxwell equations are solved in order to evaluate the absorption in thin film. Results are presented in terms of transient temperature profiles and fields for different Peclet numbers.

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

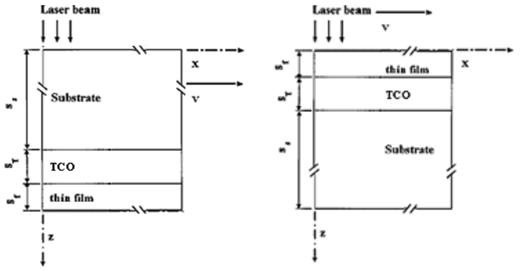
1. Introduction

The introduction of new materials and innovative processes may require the employment of high energy density sources. Lasers and electron beams are widely adopted in several material manufacturing and processing, such as welding, cutting, heat treating of metals and manufacturing of electronic components. The manufacturing of multilayer thin films deposited on glass substrate is accomplished by means of laser sources, too. Either stationary or moving localized heat sources, both continous and pulsed, irradiate the medium and provide temperature increases. The analysis of thermal conductive and optical distributions is of paramount importance to broaden the fields of applications for manufacturing. Shah et al. [1] and Tanasawa and Lior [2] carried out computational investigations of laser interactions with single and multilayer thin films on a glass substrate. Grigoropoulos [3] investigated the dependence of the thermally optical non-linearity induced in multilayer thin films because they are functions of wavelength and temperature. 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 energy absorption was taken into account by employing a thin optic model while Chen and Tien [6] examined 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]. Bianco and Manca [8] extended the analysis presented in [7] to a two-dimensional problem. Nakano et al. [9] proposed a numerical model for a thin film structure, irradiated by a circular gaussian laser beam, in which an absorbed laser power density with an exponential decay for each layer was considered in the thermal model. The effects of anisotropic thermal properties were investigated by McGahan and Cole [10]. Bianco et al. [11,12] 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 for different Peclet numbers. Bianco et al. [13] and Avagliano et al. 14] investigated the conjugate optical-thermal fields induced by laser back-scribing processes and made a comparison with front treatment ones.

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 an a-Si layer and a TCO one) is deposed on a glass substrate and it is irradiated by a Gaussian moving laser beam. The laser source irradiates the a-Si or glass surface, for front and back laser treatment respectively. Since the optical and thermal fields are strictly linked, this problem is solved by means of COMSOL Multiphysics 3.4. 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) b)

Figure 1: Sketch of the thin film and the TCO layer on glass substrate: front (a) and back treatment.

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 (s_f) layers are considered. Two configurations are investigated: back treatment (BT) in which laser spot impinges the substrate surface and front treatment (FT) where the source irradiates the a-Si surface.

Thermal and optical properties are assumed as 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 or glass surface) 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 [15], a mathematical statement of the thermal conductive problem is:

$$\frac{\partial}{\partial x}\left(k_i(T)\frac{\partial T_i}{\partial x}\right)+\frac{\partial}{\partial z}\left(k_i(T)\frac{\partial T_i}{\partial z}\right)+$$

$$+\ \dot{u}'''(T_i,x,z)=\rho c\left(\frac{\partial T_i}{\partial \theta}-v\frac{\partial T_i}{\partial x}\right) \qquad (1)$$

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:

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

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

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

or for BT cases

$$-k_f\frac{\partial T_f(x,s_f+s_t+s_s,\theta)}{\partial z}=0 \qquad (2c)$$

for $0 \le x < L_x$, θ>0

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

or for BT cases

$$-k_s\frac{\partial T_s(x,0,\theta)}{\partial z}=0 \qquad (2e)$$

for $0 \le x < L_x$, θ>0

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

or for BT cases

$$k_f\frac{\partial T_f(x,s_s+s_t,\theta)}{\partial z}=k_t\frac{\partial T_t(x,s_s+s_t,\theta)}{\partial z} \qquad (2g)$$

for $0 \le x < L_x,\ \theta > 0$

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

or for BT cases

$$k_t \frac{\partial T_t(x, s_s, \theta)}{\partial z} = k_s \frac{\partial T_s(x, s_s, \theta)}{\partial z} \quad (2i)$$

for $0 \le x < L_x,\ \theta > 0$

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

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

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

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

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 describes 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 α).

The two dimensional conductive field and the one dimensional local optical field for absorbing thin films are solved by means of the COMSOL Multiphysics 3.4 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 50 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 $x_0 = 0$. 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.

Table 1: Thermophysical properties of the employed materials

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

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

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

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 percent by doubling the mesh nodes. 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 3.4. 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 for the front laser treatment case.

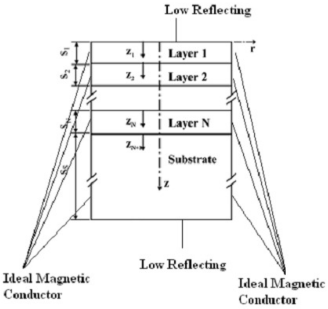


Figure 2: Thin film, TCO and glass substrate optical model for front laser treatment.

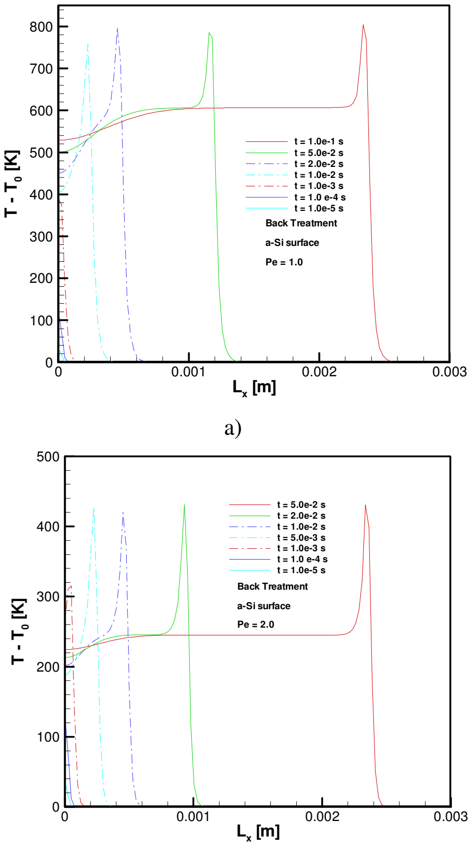
The two-dimensional heat conduction equation are solved by using the *"Heat Transfer Module"* and a "*Transient analysis"* in *"General Heat Transfer"* window for the thermal model.

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 in order to compare back and front laser treatment processes.

Figure 3 reports temperature profiles along x-direction for two different Peclet numbers in the case of back treatment, evaluated at the film surface, not directly irradiated by the laser spot. It is observed in figure 3.a that the laser spot starts to warm up the zones near the origin. At t = 1 x 10^{-2} s a maximum temperature equal to 1060 K is reached and it is localized far from origin. The highest temperature (1110 K) is detected at t = 2 x 10^{-2} s. 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) it's evident that the maximum temperatures are attained in correspondence to larger times and temperature peaks decrease. Asymptotic temperature values raises as Pe numbers decrease.

Figure 4 shows the temperature profiles for different times in the case of front treatment. It is depicted that temperature peaks and asymptotic values decrease in comparison with the back treatment simulations for Pe = 1.0 and 2.0. In fact, a maximum temperature equal to 954 K is reached at t = 2.0 x 10^{-2} s as observed in fig. 4a.



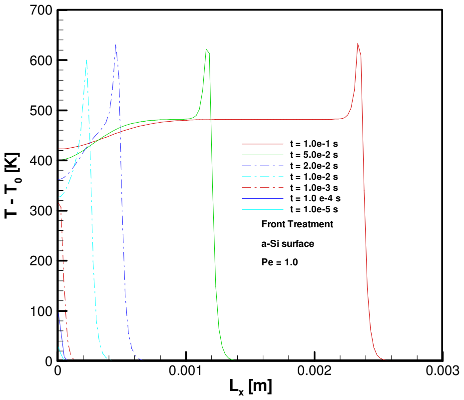
a)

b)

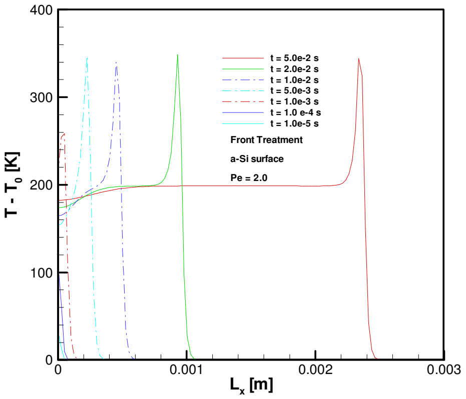
Figure 3: Temperature profiles at a-Si surface for Peclet numbers equal to 1.0 (a), 2.0 (b) at different times. Back laser treatment

Figure 5 exhibits a comparison among the temperature profiles along x-axis for different values of Peclet numbers in quasi-steady state conditions. It is observed that the smaller is the Peclet number the larger is the attained temperature. Furthermore, the zones not irradiated by the spot show more evident diffusion phenomena. As previously described, back treatment simulations reveal higher temperatures. For Pe = 1.0 a difference of about 150 K has been detected while for Pe = 5.0 there is a gap equal to 40 K.

Figure 6 depicts the temperature profiles along z-direction and x = 0.0025 m for a Peclet number of 1.0. Along the thickness of the glass, temperature increases linearly and the diffusive effect are evident while in the TCO layer temperature is almost constant. Temperature increases rapidly in the a-Si layer and reaches the value of 1085 K. Front laser treatment process exhibits lower temperatures. It is detected a peak value equal to 920 K in correspondence with the a-Si free surface, irradiated by the laser source.



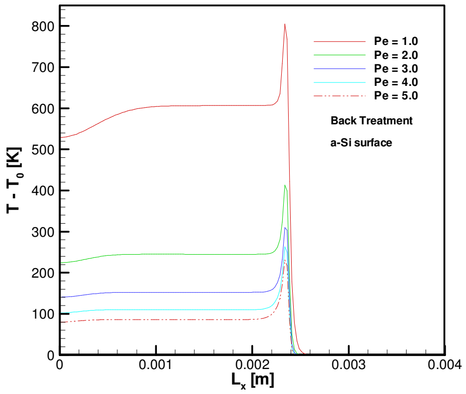
a)



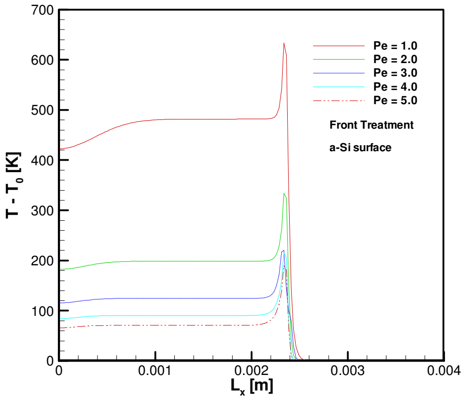
b)

Figure 4: Temperature profiles at a-Si surface for Peclet numbers equal to 1.0 (a), 2.0 (b) at different times. Front laser treatment

In Figure 7 temperature fields for Pe = 1.0 and 5.0 are reported at three different times ($1x10^{-3}$ s, $1x10^{-2}$ s and $3x10^{-2}$ s) in the case of back treatment process. For the lowest considered Peclet number (fig. 7.a), it is observed the development of the thermal affected zone inside the 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 to the conductive heat transfer because the glass is assumed as a perfect non-absorbent media.



a)



b)

Figure 5: Temperature profile along x-direction for Peclet numbers equal to 1.0, 2.0, 3.0, 4.0 and 5.0 and $x_0 = 0$; a)back laser treatment and b) front laser treatment

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 = 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 8, temperature fields are presented for Peclet numbers equal to 1.0 and 5.0 in the case of front laser treatment, for the same times as the previous figure. Comparing these fields with the previous ones, the most evident difference is the temperature drop and the heat affected zone is smaller, too.

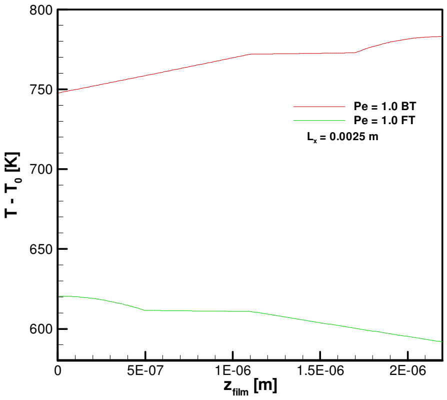


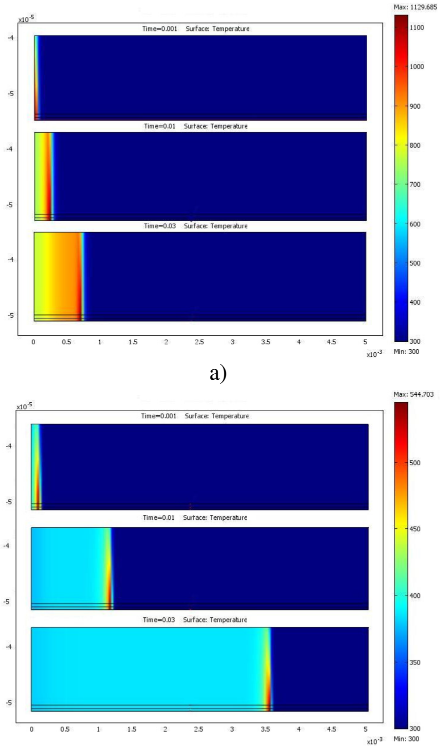
Figure 6: Temperature profiles along z-direction for Peclet number equal to 1.0 at $L_x = 0.0025$ m for back and front laser treatment processes.

5. Conclusions

A transient two-dimensional analysis of interaction between a multilayer thin film structure and a moving laser source was investigated. It was carried out numerically, by means of the COMSOL Multiphysics 3.4 code, for a semi-infinite workpiece along the heat source motion direction in order to compare back and front treatment processes. Temperature profiles and fields showed that the maximum temperature value at the quasi-steady state condition decreases at increasing Peclet number and front laser treatment reveals lower temperatures and smaller heat affected zones. The transient analysis showed that the time at which the maximum temperature is attained increased with the Peclet number.

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



a)

b)

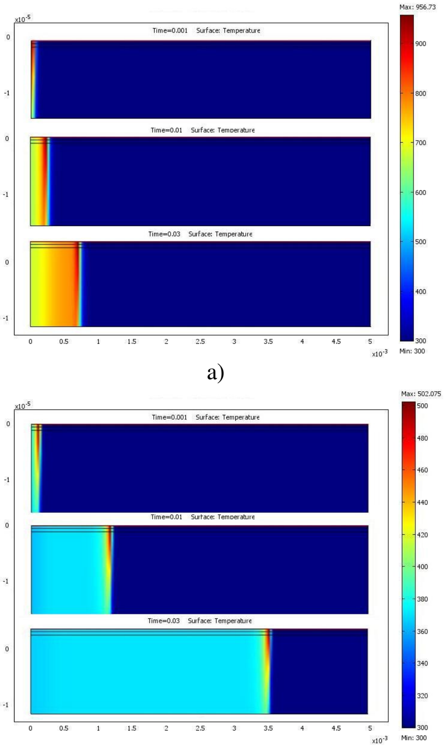
Figure 7: Temperature fields for Pe = 1.0 (a) and 5.0 (b) at $t = 1\text{x}10^{-3}$ s, $t = 1\text{x}10^{-2}$ s and $t = 3\text{x}10^{-2}$ s. Back treatment.

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



a)

b)

Figure 8: Temperature fields for Pe = 1.0 (a) and 5.0 (b) at t = 1x10^{-3}s, t = 1x10^{-2} s and t = 3x10^{-2} s. Front treatment.

7. References

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