THE THEORETICAL AND EXPERIMENTAL STUDY OF SOME METALS HEATING AND MELTING UNDER THE ACTION OF LASER RADIATION

SERGIU DINU¹, CALIN OROS¹, MARINELA VOICU¹, GABRIEL DIMA¹, CLAUDIA STIHI¹, MICHEL WAUTELET² ¹Valahia University of Targoviste, Faculty of Sciences and Arts, 28 Unirii street, Targoviste, Romania e-mail: <u>sergiudinu65@yahoo.com</u>

² University of Mons-Hainaut, Avenue Maistriau, 23, Mons, 7000, Belgium

Abstract: This study presents both theoretical and experimental results on the laser irradiation of some metals (steel, aluminium, titanium), using a Nd:YAG laser. The theoretical study involves the solving of heat equation for half-infinite targets in case that, between the thickness of target (h), the diameter of laser spot (D_s) and the thermic diffusion length (l_{th}), exists the relation $h >> D_s > l_{th}$. The determination of the temperature at the surface of the irradiated material allows quantitative estimations regarding the induced thermo-deformation and the involved phase transition, in our case, the melting. The confrontation with experience is achieved through the comparison of the thermo-deformation sizes and obtained craters and of the others related parameters with the direct microscopically measurements. The calculated values are in proper correlation with the experimental ones, the observed differences having as major cause the insufficiently precise knowledge of the involved physical values of observables, at high reached temperatures on the irradiated surfaces.

Keywords: metal, Nd:YAG laser, thermo-deformation, laser melting.

1. Experimental

The samples of steel, aluminium and titanium have cylindrical shape, with height $h \approx 5$ mm and base diameter $d \approx 20$ mm.

The characteristics of emitted radiation by Nd:YAG laser are: the wavelength $\lambda = 1,06\mu m$ (IR); the diameter of laser spot $D_s = 0,4 mm$ (steel and titanium), respectively 0.6 mm in aluminium case; the length of laser pulse $\tau_p = 3ms$ (irradiation regime is monopuls). (FWHM).

The analysis of irradiated surfaces has been done with an optical microscope whose accuracy in the estimate of the created drops (dilatations and craters) is $2\mu m$.

2. Results and discussion

The samples have been irradiated differently through the modification of pulse energy. The adequate intensities have been established with the following relation:

$$I_i = \frac{E_i}{S \cdot \tau_p} \quad , \ i = \overline{1,10} , \tag{1}$$

with $S = \pi \frac{D_s^2}{4}$ representing the area of irradiated surface and τ_p representing the laser pulse length.

The measured dimensions of formed thermodilatations (+) or craters (-), matched to the intensities given by the relation (1), are presented in the next table (tab 1):

Tabel 1. The measured dimensions of formed thermounatations (+) or craters (-)							ers (-)			
The sample	1	2	3	4	5	6	7	8	9	10
E _i (unit)	450	500	550	600	650	700	750	800	850	900
$I_i(10^9W/m^2)$	1,7	1,9	2,1	2,3	2.5	2,7	2,9	3,1	3,3	3,5
Δz_{iTi} (div)	-	-	+12	+10	+10	+13	-55	-55	-80	-120
1 div=2µm										
Δz_{isteel} (div)	-	-	+10	+22	+20	+30	-20	-30	-55	-80
1 div=2µm										
Δz_{iAl} (div)	-	-	0	0	0	-10	-15	-12	-15	-18
1 div=2µm										

Tabel 1. The measured dimensions of formed thermodilatations (+) or craters (-)

These results will be interpreted on the bases of a thermic model of interaction between the laser radiation and metallic samples.

Thus, the spatial – temporal dependence of the reached temperature in the target, T(z,t), can be established using the one-dimensional equation of heat propagation in a solid medium, whose form is:

$$\rho c \frac{\partial T}{\partial t} = K_T \frac{\partial^2 T}{\partial z^2} + \alpha A I_0 e^{-\alpha z}, \qquad (2)$$

where z is the depth in the target and t is the irradiated time. Because the laser radiation is, for the metallic sample, a superficial heat source, the solution of equation (2) has the form:

$$T(z,t) = \frac{2AI_0}{K_T} \sqrt{\chi_T \cdot t} \cdot i erfc \frac{z}{2\sqrt{\chi_T \cdot t}}.$$
(3)

For z=0 (at the sample surface) and $t=\tau_p$, the relation (3) became:

$$T(0,\tau_p) = \frac{2AI_0}{K_T} \sqrt{\chi_T \cdot \tau_p} .$$
(4)

This solution is valid in the mentioned conditions at the beginning of the article, that is: $h >> D_s > l_{th}$ (h=5 mm, $D_s=0,4$ mm, $l_{th} = \sqrt{\pi \chi_T \tau_p} / 2 = 0,12$ mm for steel; h = 5 mm, $D_s = 0,6$ mm, $l_{th} = 0,47$ mm for aluminium; h = 5mm; $D_s = 0,4$ mm; $l_{th} = 0,14$ mm for titanium.

For titanium, A=7%, $K_T=22$ J/msK, $\chi_T = \frac{K_T}{\rho c} = 0.09 \cdot 10^{-4} m^2/s$ ($\rho = 4500$ kg/m³, c=520 J/kgK), $\tau_p = 3 \cdot 10^{-3} s$, $I_{0i} \approx 0.7$ I_i, $T_{melting} = 2073$ K, $T_{vap} = 3523$ K and the relation (4) get the

$$T (0, \sigma) = 1000 E (V)$$
(5)

$$T_i(0, \tau_p) = 1900 E_i(K),$$
 (5)

with the energies E_i expressed in Joule.

form:

The correspondence between the energies E_i , expressed in units (table 1), and the energies in Joule is possible knowing that to achieve the melting temperature, $T_{melting}=2073 K$, it is necessary an energy $E_{melting}=1, IJ$, given by the formula (5), which correspond, concordant table 1, the value $E_i=750 \text{ unit}$.

A first verification of the used model is achieved calculating the superficial density of electromagnetic energy needed for the beginning of titanium sample melting:

$$W_{em \ theor} = \sqrt{\pi \rho \, c K_T \tau_p} \left(T_{melting} - T_0 \right) / 2A \,, \tag{6}$$

$$w_{emtheor} \cong 8.9 \cdot 10^6 \ J/m^2 \,. \tag{7}$$

The experimental value for the superficial density of electromagnetic energy is:

$$w_{em \exp} = \frac{E_{melting}}{S} = 8,7 \cdot 10^6 \ J / m^2,$$
(8)

close to theoretical value (7).

An additional element, that is the time needed to the laser radiation for initiate the melting process, can be calculated from:

$$t_{melting} = \frac{K_T^2 \cdot T_{melting}^2}{4A^2 I_{melting \exp}^2} = 12 \text{ ns}.$$

$$(I_{melting \exp} = \frac{E_{top}}{S\tau_p} = 2,9 \cdot 10^9 \text{ W/m}^2)$$
(9)

It may be done as well a theoretical estimation of length of the craters formed in the Ti sample based on the approximate formula:

$$\Delta z_{crater} \cong \frac{D_s}{4} \left(\frac{T_{vap}}{T_{melting}} - \frac{T_{melting}}{T_{vap}} \right).$$
(10)

Considering that the vaporization temperature of titanium is $T_{vap} = 3523$ K, it is obtained:

$$\Delta z_{crater} \cong 110 \ \mu m$$

(close to experimental value from table 1).

For steel,
$$A=27$$
 %, $K_T = 26$ J/msK, $\chi_T = \frac{K_T}{\rho c} = 6.9 \cdot 10^{-6} m^2/s$ ($\rho = 8 \cdot 10^3 kg/m^3$,

c = 470 J/kgK), $\tau_p = 3 \cdot 10^{-3} s$; $T_{melting} = 1808K$, $T_{vap} = 2573K$, $T_0 = 273K$ and, following a judgement similar to the one from the Ti case, it can be obtained:

$$w_{emtheor} = 2,73 \cdot 10^6 \ J/m^2, \tag{11}$$

$$w_{em\,\exp} = 8,7 \cdot 10^6 \ J/m^2,\tag{12}$$

$$t_{melting} = 0,9 \text{ ns},\tag{13}$$

$$\Delta z_{crater} = 72\,\mu m,\tag{14}$$

also values close to that ones with (-) sign from table 1.

Calculating the intensity of laser radiation needed for the melting induction with the formula:

$$I_{mealting} = 0.7 \frac{E_{melting}}{S\tau} = 2.9 \cdot 10^9 \, W/cm^2, \tag{15}$$

 $(E_{top} = 750 unit = 1, 1J).$

For aluminium, A=6 %, $K_T=236$ J/msK, $\chi_T = \frac{K_T}{\rho c} = 0.96 \cdot 10^{-4} \text{ m}^2/\text{s}$ ($\rho=2.71 \cdot 10^3$ kg/m³, c = 902 J/kgK), $\tau_p = 3 \cdot 10^{-3} \text{s}$, $T_{melting} = 930K$, $T_{vap} = 2543K$, $T_0 = 273K$. It results:

$$w_{emtheor} = 12,7 \cdot 10^6 \ J/m^2,\tag{16}$$

$$w_{emexp} = 3.6 \cdot 10^6 \ J/m^2 \,, \tag{17}$$

$$t_{melting} = 2,3 \ \mu s, \tag{18}$$

$$\Delta z_{crater} = 350\,\mu m \tag{19}$$

$$(I_{melting exp} = \frac{E_{melting}}{S\tau_p} = 1.2 \cdot 10^9 W / m^2).$$

Thermodilatations of the Al surface were not observed at intensities lower then the melting limit.

Another confrontation with the experience is possible, in the case of steel and Ti, from the estimation of the linear dimensions of the thermodilatation, based on the linear dilatation and the comparison of these with the measurements realized using optical microscope (table 1, values with "+"). Thus, considering the length dilatation of the cylinder with l_{\perp} high and $S = \pi \frac{D_s^2}{s}$ has area, it may be written:

with l_{th} high and $S = \pi \frac{D_s^2}{4}$ base area, it may be written:

$$\Delta z_{i\,theor} = \alpha z_0 \Delta T_i \,, \tag{21}$$

where $z_0 \approx l_{th} = 0.12 \text{ mm}$ and $\alpha = 1.2 \cdot 10^{-5} \text{ K}^{-1}$ for steel and for Ti, the values are $z_0 = 0.14 \text{ mm}$ and $\alpha = 1.08 \cdot 10^{-5} \text{ K}^{-1}$ ($\Delta T_i \cong T_i - T_0$, with $T_0 = 273 \text{ K}$.

The results are mentioned in the next tables (table 2 and table 3):

The second (steel)	1	C	2	4	5	6
The sample (steel)	1	2	3	4	3	0
$T_{i}(K)$	1090	1208	1327	1453	1572	1690
$\Delta z_{iteor} (\mu m)$	1,17	1,34	1,51	1,69	1,87	2,04
$\Delta z_{iexp}(\mu m)$	0	0	+25	+35	+30	+50

Table 2. Theoretical and experimental results of steel thermodilatations

Table 3. Theoretical and experimental results of titanium thermodilatations

The sample (Ti)	1	2	3	4
$T_{i}(K)$	1515	1650	1805	1940
$\Delta z_{i \text{ teor}} (\mu m)$	1,87	2,08	2,31	2,52
$\Delta z_{iexp}(\mu m)$	+15	+15	+22	+30

An interesting element is related to the comparison, using microscope, of the thermodilatation form with that of the intensity distribution in the laser beam (Figure 1). This suggests the fact that in the central zone of the beam, because of the higher values, the reached temperature in the spot center is higher, therefore the dilatation extend will be higher too.

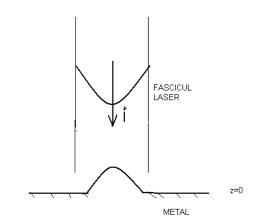


Fig. 1. The comparison of thermodilatation form with that of intensity distribution in the laser beam.

3. Conclusions

It has been possible to observe an approach close enough to the theoretical results with the experimental ones, specially in the determination of the superficial density of the needed energy for induction of titanium melting, of the fusion depth (better concordances has been observed at steel and Ti) and even of the critical laser intensity in order to reach of the melting limit (at steel and Ti).

For aluminium, the concordances between theoretical and experimental results are not very good, a possible reason being that the Al surface, in contact with the air, transforms in Al_2O_3 .

This suggests that, although the values of the involved physical parameters, in calculations, are insufficiently known, specially at high temperature reached at the samples surfaces, the used thermic model for estimating the shown up thermo dilatation after the irradiation was not suitable, but the explanation is simple: the dilated and warmed volume is much more higher then the considerate one in the application of the thermic dilatation law, fact that appreciably minimizes the theoretical values of the dilatation at the samples surfaces.

Finally, it is obtained that the necessity of the continuation of this type of experiences even in other metals case for more precise estimations on the used theoretical model.

References

[1] Diebold, U., Surf. Sci. Rep., 48, 53, 2003.

[2] Le Mercier, T., Mariot, J-M., Parent, P., Fontaine, M-F., Hague, C. F., Quarton, M., Appl. Surf. Sci. 86 382, 1995.

[3] Robert, T.D., Laude, L.D., Geskin, V.M., Lazzaroni, R., Gouttebaron, R., *Thin Solid Films* 440, 268, 2003.

[4] Bauerle, D., Laser processing and chemistry, Springer, Berlin, 2000.

[5] Ursu, I., Prokhorov, A., Interacția radiației laser cu substanța, Ed.Academiei RSR, București, 1986.

[6] Palik, E.D., Handbook of Optical Constants of Solids, Academic Press, Orlando, 1985.

[7] Weast, R.C., *CRC Handbook of Chemistry and Physics*, 67th edition (CRC Press, Boca Raton, 1986).

[8] Wautelet, M. and Gehain, E.D., Semicond. Sci. Technol. 5, 246, 1990.

[9] Van Overschelde, O., Dinu, S., Guisbiers, G., Monteverde, F., Nouvellon, C., Wautelet, M., *Applied Surface Science*, 252, 4722 – 4727, 2006.

[10] Wautelet, M., Quenon, P., Jardin, A., Semic. Sci. Technol.3, 54-59, 1988.

THE MONITORING OF 2D-3D TRANSITION FOR InAs/GaAs (001) SELF-ASSEMBLED QUANTUM DOTS BY ATOMIC FORCE MICROSCOPY

OANA BUTE¹, VALERICA GH. CIMPOCA¹, ERNESTO PLACIDI², FABRIZIO ARCIPRETE²

¹*Valahia* University of Targoviste, Physics Department, Science and Arts Faculty, 2 Carol I street, 130024, Targoviste, Romania. E-mail: <u>oanab@valahia.ro</u>

² Universita degli Studi di Roma Tor Vergata, Via della Ricerca Scientifica, 1, 00133 Roma, Italy

Abstract. We present a detailed Atomic Force Microscopy study of InAs/GaAs (001) selfassembled quantum dots grown by Molecular Beam Epitaxy during its complete evolution cycle (transition from 2D islands to 3D islands). We have performed a statistical analysis regarding quantum dot number density, identifying the existence of two separated distributions (for quasi-3D dots and 3D dots). We have observed that the density number value of quasi-3D QDs decreases from 1.1 x 10^{10} cm⁻² to 4.3 x 10^{9} cm⁻² for a coverage between 1.57 ML and 1.61 ML, while for 3D QDs it increases by a factor of 10 (from 2.1 x 10^{10} cm⁻² to 2.3 x 10^{10} cm⁻²) so as the 3D QDs become the prevailed structures. We can assume as critical coverage, 1.59 ML.

1. Introduction.

The general importance and desirability for advancement of technology requires high degree of control of composition, size and structure. This is so critical to the area of nanostructures synthesis that self-assembly has been an increasing hallmark of this field. The growth of lattice-mismatch semiconductor systems such as InAs|GaAs has been known to produce structures as 3D islands by Stranski-Krastanow (SK) mode.

Typically, such islands don't form immediately on the substrate. In the first stage of the growth, a pseudomorphic thin layer is created which is elastically distorted. This pseudomorphic layer is named wetting layer (WL) and the islands form, practically, on its top.

The driving force for the self-assembly process during heteroepitaxial growth (the case of GaAs and InAs, the most commonly used pair of compounds) is the misfit between the crystal lattice of the growing layer and that of the substrate. This misfit of lattice constants is