PROGRESS IN ELECTRICAL ENGINEERING
Vol. 1, No. 2, 2020, 231-239

URL : www.arfjournals.com

On Analytical Approach for Prognosis of Growth of Films by using Pulsed Laser Deposition. Influence of Parameters on Technological Processes

E.L. Pankratov

[1]*Nizhny Novgorod State University, 23 Gagarin avenue, Nizhny Novgorod, 603950, Russia*
[2]*Nizhny Novgorod State Technical University, 24 Minin Street, Nizhny Novgorod, 603950, Russia*
E-mail: elp2004@mail.ru

Received: 13 August 2020 / Revised: 25 September 2020 / Accepted: 23 October 2020 / Published: 28 December 2020

Abstract: In this paper, we consider an analytical approach for analyzing film growth by pulsed laser deposition. The influence of the parameters of the growth process on the growth of films is investigated.

Keywords: growth of films; pulsed laser deposition; analytical approach for modeling.

INTRODUCTION

One of the most promising modern methods for producing epitaxial layers is pulsed laser deposition. This method gives a possibility to growth special materials (metals, carbides, etc.) to the surface of parts, which allows you to restore geometry, increase surface strength and corrosion resistance, etc. [1-10]. In this work we consider mass and heat transfer in the reaction chamber during the growth of an epitaxial layer using pulsed laser deposition. An analytical approach for analyzing the considered processes was introduced, which allows one to take into account their nonlinearity, as well as changes in parameters in space and time.

METHOD OF SOLUTION

To solve our aims, we consider one-dimensional mass and heat transfer in the direction, which is perpendicular to the source of material evaporated during laser deposition (see Fig. 1). We describe the heat transfer using the second Fourier law

$$c_p\rho\left[\frac{\partial T(x,t)}{\partial t}-u(t)\frac{\partial T(x,t)}{\partial x}\right]=\frac{\partial}{\partial x}\left[\lambda(T)\frac{\partial T(x,t)}{\partial x}\right]+p(x,t), \tag{1}$$

where ρ is the density of the evaporated material; c_p is the specific heat at constant pressure; $\lambda(T)$ is the thermal conductivity; $p\,(x,t)$ is the power density of laser radiation; x and t are the current coordinate and time; $T\,(x,t)$ is the heating temperature of the material. The temperature dependence of the thermal conductivity coefficient in the desired temperature range can be approximated as follows: $\lambda\,(T) = \lambda_{ass}\{1+\mu\,[T_d/T(x, t)]^{\varphi}\}$ (see, for example, [11]); $\alpha\,(T) = \lambda\,(T)/c\,(T)$ is the thermal diffusivity. The speed of movement of the evaporation boundary is determined by the flows J_i of particles evaporated from the surface: $u\,(t) = \sum_i J_i/\rho_i$, where i - means the material used during growth. The boundary and initial conditions could be written in the following form

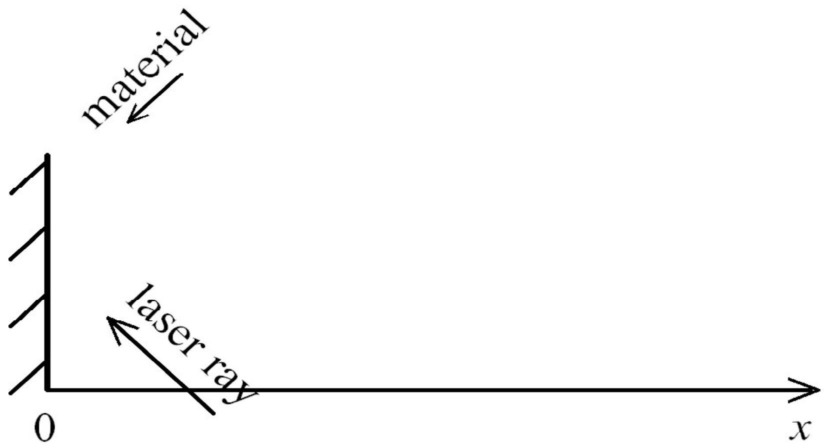

Figure 1: The direction of motion of the material vaporized during laser deposition

$$\lambda \left.\frac{\partial T(x,t)}{\partial x}\right|_{x=0} = Q_p \cdot u(t),\ \mathrm{T}\ (¥,\mathrm{t}) = \mathrm{T}_r,\ \mathrm{T}\ (\mathrm{x},0) = \mathrm{T}_r. \tag{1a}$$

Here T_r is the equilibrium temperature equals room temperature; Q_p is the heat of vaporization. We describe the transfer of the growth components using the second Fick law in the following form

$$\frac{\partial C(x,t)}{\partial t} - u(t)\frac{\partial C(x,t)}{\partial x} = \frac{\partial}{\partial x}\left[D_C \frac{\partial C(x,t)}{\partial x}\right] \tag{2}$$

with boundary and initial conditions

$$\mathrm{C}\ (0,\ \mathrm{t}) = \mathrm{C}_0,\ \mathrm{C}\ (\infty,\ \mathrm{t}) = 0,\ \mathrm{C}\ (0,\ 0) = \mathrm{C}_0,\ \mathrm{C}\ (\mathrm{x} > 0,\ 0) = 0, \tag{2a}$$

where $C(x,t)$ is the concentration of vaporized material; D_C is the diffusion coefficient of this material.

Next, we transform equations (1) and (2) to the following integro-differential forms, taking into account the boundary and initial conditions (1a) and (2a)

$$T(x,t)=T(x,t)+\frac{\lambda_{ass}}{c_p\rho L}\int_0^t\left[1+\frac{\mu T_d}{T(x,\tau)}\right]^{\varphi}\frac{\partial T(x,\tau)}{\partial x}d\tau+\frac{1}{c_p\rho L}\int_0^t\int_0^x p(v,\tau)dvd\tau-$$

$$-\frac{c_p\rho}{L}\left\{\int_0^x\left[T(v,t)-T_r\right]dv-\int_0^t u(\tau)T(x,\tau)d\tau\right\}-\frac{u(t)Q_p}{c_p\rho L}-\frac{u(t)Q_m}{c_p\rho L},\tag{1a}$$

$$C(x,t)=C(x,t)+\frac{1}{L^2}\int_0^t D_C C(x,\tau)d\tau-\frac{1}{L^2}\int_0^t\int_0^x C(v,\tau)\frac{\partial D_C}{\partial v}dvd\tau+C_0+\frac{C_0}{L^2}\int_0^t D_C d\tau-$$

$$-\frac{1}{L^2}\int_0^x(x-v)C(v,t)dv+\frac{1}{L^2}\int_0^t u(\tau)\int_0^x C(v,\tau)dvd\tau.\tag{2b}$$

Here Q_m is the heat of melting; L is the distance between the source of growth material and the grown layer. Now we solve equations (1b) and (2b) using the method of averaging functional corrections [12]. Framework this method, we replace the unknown functions $T(x,t)$ and $C(x,t)$ by their unknown average values α_{1T} and α_{1C} in the right-hand sides of the considered equations. Then we obtain the equations for the first approximations of the desired functions $T_1(x,t)$ and $C_1(x,t)$

$$T_1(x,t)=\alpha_{1T}-\frac{c_p\rho}{L}\left[(\alpha_{1T}-T_r)x-\alpha_{1T}\int_0^t u(\tau)d\tau\right]+$$

$$+\frac{1}{c_p\rho L}\int_0^t\int_0^x p(v,\tau)dvd\tau-\frac{u(t)Q_p}{c_p\rho L}-\frac{u(t)Q_m}{c_p\rho L},\tag{3a}$$

$$C_1(x,t)=\alpha_{1C}+\frac{\alpha_{1C}}{L^2}\int_0^t D_C d\tau-\frac{\alpha_{1C}}{L^2}\int_0^t\int_0^x\frac{\partial D_C}{\partial v}dvd\tau+$$

$$+C_0+\frac{C_0}{L^2}\int_0^t D_C d\tau-\alpha_{1C}\frac{x^2}{2L^2}+x\frac{\alpha_{1C}}{L^2}\int_0^t u(\tau)d\tau.\tag{3b}$$

The unknown average values of a_{1T} and a_{1C} are determined using standard relations [12]

$$\alpha_{1T}=\frac{1}{\Theta L}\int_0^{\Theta}\int_0^{L}T_1(x,t)\,d\,x\,d\,t, \tag{4a}$$

$$\alpha_{1C}=\frac{1}{\Theta L}\int_0^{\Theta}\int_0^{L}C_1(x,t)\,d\,x\,d\,t. \tag{4b}$$

Substitution relations (3) into relations (4) and calculating of the appropriate integrals leads to relations for average values of α_{1T} and α_{1C}

$$\alpha_{1T}=\left[T_r\frac{c_p\rho}{2}+\frac{1}{\Theta L c_p\rho L}\int_0^{\Theta}(\Theta-t)\int_0^{L}(L-x)\,p(x,t)\,d\,x\,d\,t-\frac{Q_p}{c_p\rho L\Theta}\int_0^{\Theta}u(t)\,d\,t-\right.$$

$$\left.-\frac{Q_m}{c_p\rho L\Theta}\int_0^{\Theta}u(t)\,d\,t\right]\Bigg/c_p\rho\left[\frac{1}{2}-\frac{1}{\Theta L}\int_0^{\Theta}(\Theta-t)\,u\,(t)\,d\,t\right], \tag{5a}$$

$$\alpha_{1C}=\left[C_0+\frac{C_0}{\Theta L^3}\int_0^{\Theta}(\Theta-t)\int_0^{L}D_C\,d\,x\,d\,t\right]\Bigg/\left[\frac{1}{\Theta L^3}\int_0^{\Theta}(\Theta-t)\int_0^{L}(L-x)\frac{\partial D_C}{\partial v}\,d\,x\,d\,t-\right.$$

$$\left.-\frac{1}{\Theta L^3}\int_0^{\Theta}(\Theta-t)\int_0^{L}D_C\,d\,x\,d\,t+\frac{1}{6}-\frac{1}{2\Theta L}\int_0^{\Theta}(\Theta-t)\,u(t)\,d\,t\right]. \tag{5b}$$

The second-order approximations of the required functions $T\,(x,t)$ and $C\,(x,t)$ have been determined framework standard procedure [12], i.e. by replacing these functions by the following sums: $T\,(x,t)\to\alpha_{2T}+T_1(x,t)$ и $C\,(x,t)\to\alpha_{2C}+C_1(x,t)$ on the right side of equations (2), where α_{2T} and α_{2C} are the average values of the second-order approximations of the considered temperature $T_2(x,t)$ and concentration $C_2(x,t)$. Higher-order approximations are calculated similarly with a corresponding increase in the summation indices indicating the order of approximation. The relations for the second-order approximations of the considered functions after the considered substitution take the following form

$$T_2(x,t)=\alpha_{2T}+T_1(x,t)-\frac{c_p\rho}{L}\left\{\int_0^{x}\left[\alpha_{2T}+T_1(v,t)-T_r\right]d\,v-\int_0^{t}u\,(\tau)\left[\alpha_{2T}+T_1(x,\tau)\right]d\,\tau\right\}+ \tag{6a}$$

$$+\frac{\lambda_{ass}}{c_p\rho L}\int_0^{t}\frac{\partial\,T_1(x,\tau)}{\partial\,x}\left[1+\frac{\mu\,T_d}{\alpha_{2T}+T_1(x,\tau)}\right]^{\varphi}d\,\tau+\frac{1}{c_p\rho L}\int_0^{t}\int_0^{x}p(v,\tau)\,d\,v\,d\,\tau-\frac{u(t)\,Q_p}{c_p\rho L}-\frac{u(t)\,Q_m}{c_p\rho L},$$

$$C_2(x,t)=\alpha_{2C}+C_1(x,t)+\frac{1}{L^2}\int_0^t D_C[\alpha_{2C}+C_1(x,\tau)]d\tau-\frac{1}{L^2}\int_0^t\int_0^x[\alpha_{2C}+C_1(v,\tau)]\frac{\partial D_C}{\partial v}d v d\tau+$$

$$+\frac{C_0}{L^2}\int_0^t D_C d\tau-\frac{1}{L^2}\int_0^x(x-v)[\alpha_{2C}+C_1(v,t)]d v+C_0+\frac{1}{L^2}\int_0^t u(\tau)\int_0^x[\alpha_{2C}+C_1(v,\tau)]d v d\tau. \quad (6b)$$

Calculation of the considered average values of the second-order approximations of the required functions α_{2T} and α_{2C} is carried out using standard relations [12]

$$\alpha_{2T}=\frac{1}{\Theta L}\int_0^\Theta\int_0^L[T_2(x,t)-T_1(x,t)]d x d t, \quad (7a)$$

$$\alpha_{2C}=\frac{1}{\Theta L}\int_0^\Theta\int_0^L[C_2(x,t)-C_1(x,t)]d x d t. \quad (7b)$$

leads to the following equations for the considered parameters

$$\frac{c_p\rho}{L}\int_0^\Theta(\Theta-t)\int_0^L u(t)[\alpha_{2T}+T_1(x,t)]d x d t-\frac{c_p\rho}{L}\int_0^\Theta\int_0^L(L-x)[\alpha_{2T}+T_1(v,t)-T_r]d x d t-$$

$$-\frac{Q_p}{c_p\rho}\int_0^\Theta u(t)d t+\frac{\lambda_{ass}}{c_p\rho L}\int_0^\Theta(\Theta-t)\int_0^L\frac{\partial T_1(x,t)}{\partial x}\left[1+\frac{\mu T_d}{\alpha_{2T}+T_1(x,t)}\right]^\varphi d x d t+\int_0^\Theta(\Theta-t)\int_0^L(L-x)\times$$

$$\times p(x,t)d x d t-Q_m\int_0^\Theta u(t)d t\Big/c_p\rho=0, \quad (8a)$$

$$\int_0^\Theta(\Theta-t)\int_0^L D_C[\alpha_{2C}+C_1(x,t)]d x d t-\int_0^\Theta(\Theta-t)\int_0^L(L-x)[\alpha_{2C}+C_1(x,t)]\frac{\partial D_C}{\partial v}d x d t+C_0L^3\Theta+$$

$$+\int_0^\Theta(\Theta-t)u(t)\int_0^L(L-x)[\alpha_{2C}+C_1(x,t)]d x d t-L^2\int_0^\Theta\int_0^L(L-x)^2[\alpha_{2C}+C_1(x,t)]d x d t+$$

$$+C_0\int_0^\Theta(\Theta-t)\int_0^L D_C d x d t=0. \quad (8b)$$

Average value α_{2C} could be determined by relation (9)

$$\alpha_{2C}=\left[\int_0^\Theta(\Theta-t)\int_0^L(L-x)C_1(x,t)\frac{\partial D_C}{\partial v}d x d t-\int_0^\Theta(\Theta-t)\int_0^L D_C C_1(x,t)d x d t-C_0\int_0^\Theta(\Theta-t)\times\right.$$

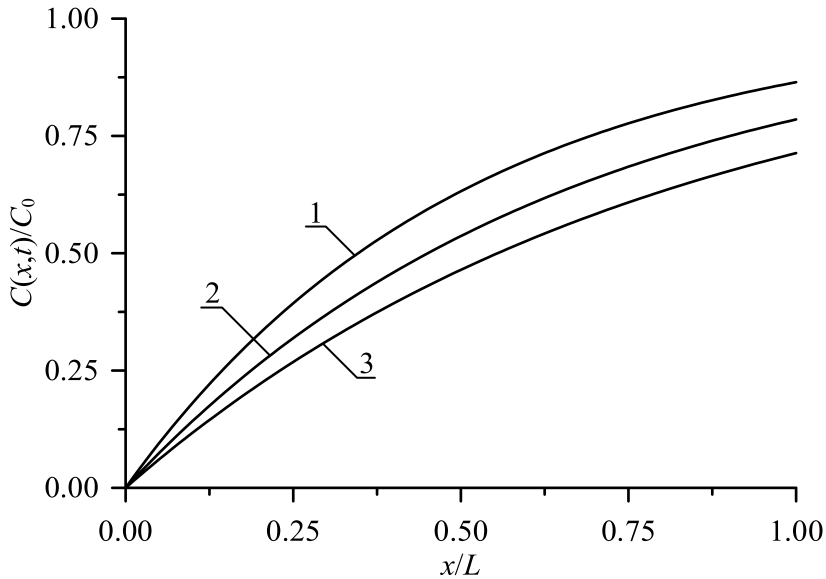

Figure 2: Distributions of the concentration of the growth component at various values of the laser pulse power. Increasing of curve number corresponds to increasing of the pulse power

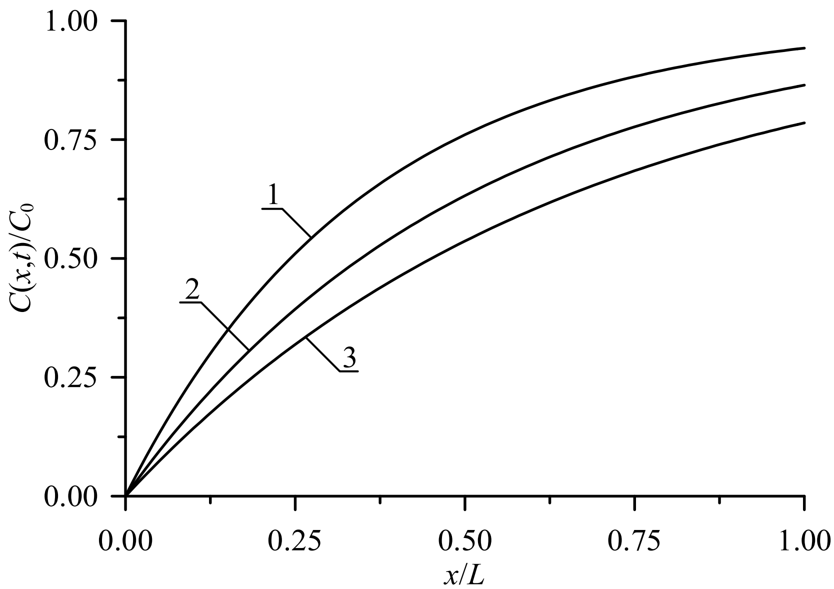

Figure 3: Distributions of the concentration of the growth component at various values of the laser pulse continuance. Increasing of curve number corresponds to increasing of the pulse continuance

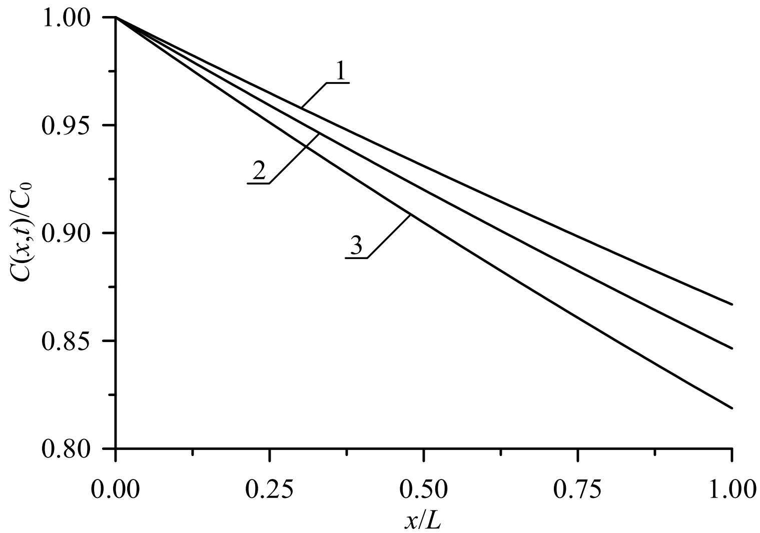

Figure 4: Distributions of the concentration of the growth component at various values of the distance between source of the growth component and epitaxial layer. Increasing of curve number corresponds to increasing of the distance

$$\times\int_0^L D_C\,d\,x\,d\,t+L^2\int_0^{\Theta}\int_0^L (L-x)^2 C_1(x,t)\,d\,x\,d\,t-\int_0^{\Theta}(\Theta-t)\,u(t)\int_0^L (L-x)C_1(x,t)\,d\,x\,d\,t-C_0L^3\Theta\Bigg]\times$$

$$\times\left[\int_0^{\Theta}(\Theta-t)\int_0^L D_C\,d\,x\,d\,t-\int_0^{\Theta}(\Theta-t)\int_0^L (L-x)\frac{\partial D_C}{\partial v}\,d\,x\,d\,t+\int_0^{\Theta}(\Theta-t)u(t)\int_0^L (L-x)\,d\,x\,d\,t-\right.$$

$$\left.-\Theta L^5/3\right]^{-1}. \tag{9}$$

The average value of α_{2T} depends on the value of parameter φ and calculated with account available empirical data. In this paper we analyzed the spatio-temporal distributions of the concentration of the growth component and temperature was carried out analytically by using the second-order approximation framework the method of averaging functional corrections. The approximation is usually sufficient to make a qualitative analysis and obtain some quantitative results. The results of analytical calculations were verified by comparing them with the results of numerical modeling.

DISCUSSION

Let us analyze the spatio-temporal distribution of the concentration of the growth component. Figures 2 and 3 show the dependences of the concentration of the growth component on the power and duration of the laser pulse for a fixed value of another parameter. An increasing of the concentration is natural, because with an increasing the power and continuance of the laser pulse, it leads to an increase in the amount of evaporated material. In fig. Figure 4 shows the dependences of the concentration of the growth component on the distance between the source of growth material and the grown layer. This concentration may decrease due to loss of material beyond the surface of the substrate (the concentration was considered within the direction from the target to the substrate).

CONCLUSIONS

In this paper, we consider an analytical approach for analyzing film growth by pulsed laser deposition. The influence of the parameters of the growth process on the growth of films is investigated.

REFERENCES

[1] A. Nutsch, B. Dahlheimer, N. Dohr, H. Kratzer, R. Lukas, B. Torabi, G. Trankle, G. Abstreiter, G. Weimann. Chemical beam epitaxy of integrated 1.55 mu m lasers on exact and misoriented (100)-InP substrates. *J. Crystal Growth.* **Vol. 188**. P. 275-280 (1998).

[2] E.V. Chelnokov, N. Bityurin, I. Ozerov, W. Marine. Two-photon pumped random laser in nanocrystalline ZnO. *Appl. Phys. Lett.* **Vol. 89**. Paper No. 171119 (2006).

[3] W.P. Shen, H.S. Kwok. Crystalline phases of II-VI compound semiconductors grown by pulsed laser deposition. *Appl. Phys. Lett.* **Vol. 65**. P. 2162-2164 (1994).

[4] A.N. Zherikhin, A.I. Khudobenko, R.T. Willyams, D. Vilkinson, K.B. Ucer, G. Hiong, V.V. Voronov. Laser deposition of ZnO films on silicon and sapphire substrates. *Quantum electronics.* **Vol. 33** (11). P. 975-980 (2003).

[5] K. Abe, O. Eryu, S. Nakashama, M. Terai, M. Kubo, M. Niraula, K. Yasuda. Optical emission characteristics of ablation plasma plumes during the laser-etching process of CdTe. *J. Electron. Mater.* **Vol. 34**. P. 1428-1431 (2005).

[6] J. Bonse, J.M. Wrobel, J. Krüger, W. Kautek. Ultrashort-pulse laser ablation of indium phosphide in air. *Appl. Phys. A.* **Vol. 72**. P. 89-94 (2001).

[7] M. Couillard, A. Borowiec, H.K. Haugen, J.S. Preston, E.M. Griswold, G.A. Botton. Subsurface modifications in indium phosphide induced by single and multiple femtosecond laser pulses: A study on the formation of periodic ripples. *J. Appl. Phys.* **Vol. 101**. Paper No. 033519 (2007).

[8] S.P. Zhvavyi, G.L. Zykov. Simulation of dynamics of phase transitions in CdTe by pulsed laser irradiation. *Appl. Surf. Sci.* **Vol. 253**. P. 586-591 (2006).

[9] A. Borowiec, H.K. Haugen. Subwavelength ripple formation on the surfaces of compound semiconductors irradiated with femtosecond laser pulses. *Appl. Phys. Lett.* **Vol. 82**. P. 4462-4464 (2003).

[10] J. Bonse, S.M. Wiggins, J. Solis. Dynamics of phase transitions induced by femtosecond laser pulse irradiation of indium phosphide. *Appl. Phys. A.* **Vol. 80**. P. 243-248 (2005).

[11] K.V. Shalimova. *Physics of semiconductors*. Moscow: Energoatomizdat, 1985.

[12] Yu.D. Sokolov. Applied mechanics. **Vol. 1** (1). P. 23-35 (1955).