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ON PROGNOSIS OF GROWTH OF FILM BY PULSED LASER DEPOSITION AND INFLUENCE OF VARIATION OF PARAMETERS ON TECHNOLOGICAL PROCESS

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Abstract

In this paper, we consider an analytical approach for analyzing film growth by pulsed laser deposition. The approach gives a possibility to analyzed the considered technological in more common case. The influence of the parameters of the growth process on the growth of films is investigated.

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1. 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.

2. 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 Figure 1).

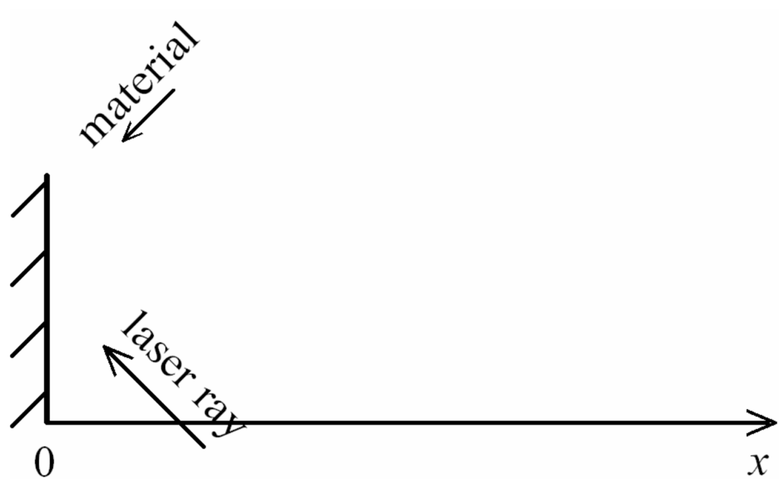

Figure 1. The direction of motion of the material vaporized during laser deposition.

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:

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

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

$$C(0,t)=C_0,\ C(\infty,t)=0,\ C(0,0)=C_0,\ C(x>0,0)=0, \tag{2a}$$

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)

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

$$+ \frac{1}{c_p \rho L} \int_0^t \int_0^x p(v,\ \tau) dv d\tau - \frac{c_p \rho}{L} \left\{ \int_0^x [T(v,\ t) - T_r] dv \right.$$

$$\left. - \int_0^t u(\tau) T(x,\ \tau) d\tau \right\} - \frac{u(t) Q_p}{c_p \rho L} - \frac{u(t) Q_m}{c_p \rho L}, \quad (1b)$$

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

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

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

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 $C_1(x,\ t)$

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

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

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

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

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

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

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

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

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

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

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

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

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: $T(x, t) \to \alpha_{2T} + T_1(x, t)$ and $C(x, t) \to \alpha_{2C} + C_1(x, t)$ 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:

$$T_2(x, t) = \alpha_{2T} + T_1(x, t)$$

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

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

$$+ \frac{1}{c_p \rho L} \int_0^t \int_0^x p(v, \tau) dv d\tau - \frac{u(t) Q_p}{c_p \rho L} - u(t) Q_m / c_p \rho L, \qquad (6a)$$

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

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

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

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

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]

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

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

leads to the following equations for the considered parameters:

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

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

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

$$+ \int_0^{\Theta}(\Theta - t)\int_0^{L}(L - x)p(x, t)dxdt - Q_m\int_0^{\Theta}u(t)dt/c_p\rho = 0, \tag{8a}$$

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

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

$$+ C_0 L^3 \Theta + \int_0^\Theta (\Theta - t) u(t) \int_0^L (L - x)[\alpha_{2C} + C_1(x, t)] dxdt$$

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

$$+ C_0 \int_0^\Theta (\Theta - t) \int_0^L D_C dxdt = 0. \tag{8b}$$

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

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

$$- \int_0^\Theta (\Theta - t) \int_0^L D_C C_1(x, t) dxdt - C_0 \int_0^\Theta (\Theta - t) \int_0^L D_C dxdt$$

$$+ L^2 \int_0^\Theta \int_0^L (L - x)^2 C_1(x, t) dxdt$$

$$\left. - \int_0^\Theta (\Theta - t) u(t) \int_0^L (L - x) C_1(x, t) dxdt - C_0 L^3 \Theta \right]$$

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

$$\left. + \int_0^\Theta (\Theta - t) u(t) \int_0^L (L - x) dxdt - \Theta L^5 / 3 \right]^{-1}. \tag{9}$$

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 modelling.

3. 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 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).

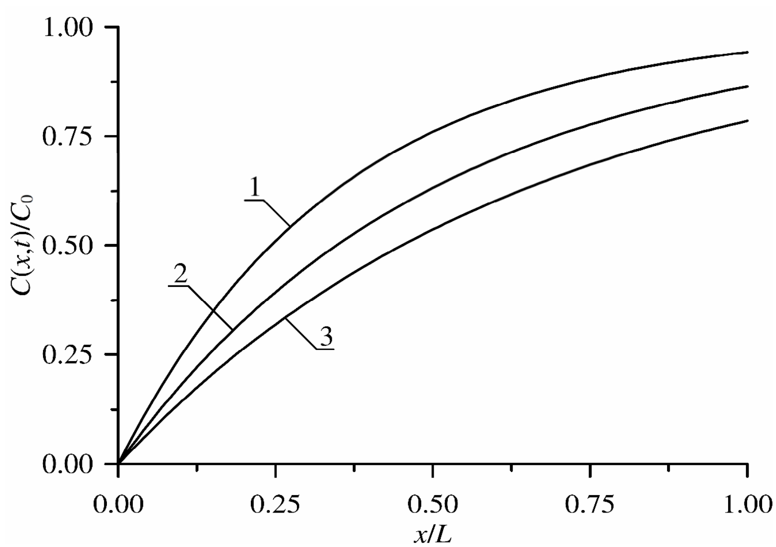

Figure 2. Distributions of the concentration of the growth component at various values of the laser pulse power. Increasing of curve number corresponds to increasing of the pulse power.

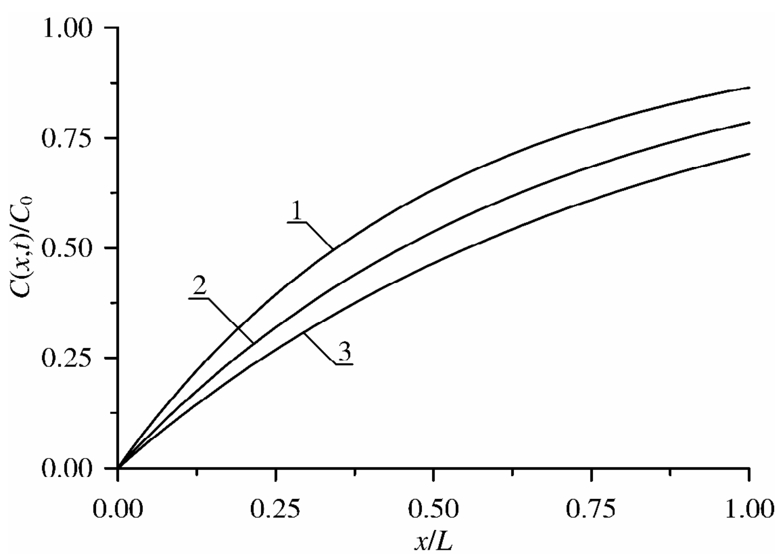

Figure 3. Distributions of the concentration of the growth component at various values of the laser pulse continuance. Increasing of curve number corresponds to increasing of the pulse continuance.

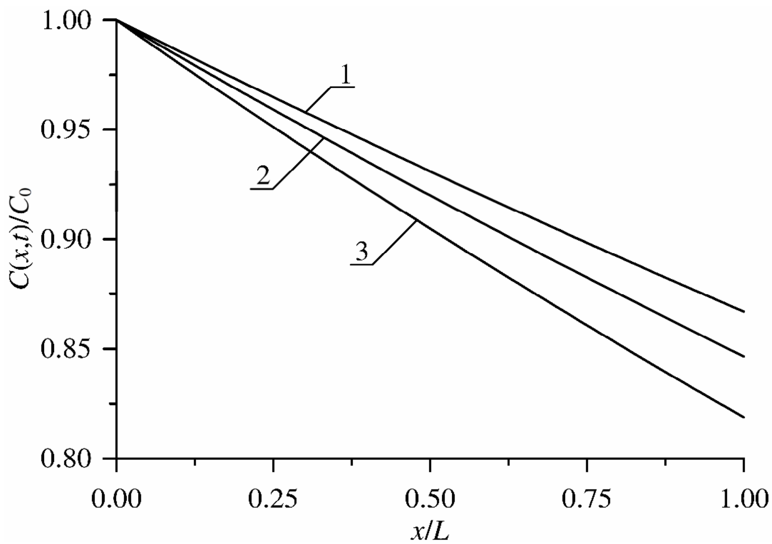

Figure 4. Distributions of the concentration of the growth component at various values of the distance between source of the growth component and epitaxial layer. Increasing of curve number corresponds to increasing of the distance.

4. Conclusion

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 and G. Weimann, Chemical beam epitaxy of integrated 1.55μm lasers on exact and misoriented (100)-InP substrates, Journal of Crystal Growth 188(1-4) (1998), 275-280.

DOI: https://doi.org/10.1016/S0022-0248(98)00073-6

[2] E. V. Chelnokov, N. Bityurin, I. Ozerov and W. Marine, Two-photon pumped random laser in nanocrystalline ZnO, Applied Physics Letters 89(17) (2006); Article 171119.

DOI: https://doi.org/10.1063/1.2370879

[3] W. P. Shen and H. S. Kwok, Crystalline phases of II-VI compound semiconductors grown by pulsed laser deposition, Applied Physics Letters 65(17) (1994); Article 2162.

DOI: https://doi.org/10.1063/1.112749

[4] A. N. Zherikhin, A. I. Khudobenko, R. T. Willyams, J. Wilkinson, K. B. User, G. Xiong and V. V. Voronov, Laser deposition of ZnO films on silicon and sapphire substrates, Quantum Electronics 33(11) (2003), 975-980.

DOI: https://doi.org/10.1070/QE2003v033n11ABEH002533

[5] K. Abe, O. Eryu, S. Nakashima, M. Terai, M. Kubo, M. Niraula and K. Yasuda, Optical emission characteristics of ablation plasma plumes during the laser-etching process of CdTe, Journal of Electronic Materials 34(11) (2005), 1428-1431.

DOI: https://doi.org/10.1007/s11664-005-0201-7

[6] J. Bonse, J. M. Wrobel, J. Kruger and W. Kautek, Ultrashort-pulse laser ablation of indium phosphide in air, Applied Physics A 72(1) (2001), 89-94.

DOI: https://doi.org/10.1007/s003390000596

[7] M. Couillard, A. Borowiec, H. K. Haugen, J. S. Preston, E. M. Griswold and G. A. Botton, Subsurface modifications in indium phosphide induced by single and multiple femtosecond laser pulses: A study on the formation of periodic ripples, Journal of Applied Physics 101(3) (2007); Article 033519.

DOI: https://doi.org/10.1063/1.2423136

[8] S. P. Zhvavyi and G. L. Zykov, Simulation of dynamics of phase transitions in CdTe by pulsed laser irradiation, Applied Surface Science 253(2) (2006), 586-591.

DOI: https://doi.org/10.1016/j.apsusc.2005.12.116

[9] A. Borowiec and H. K. Haugen, Subwavelength ripple formation on the surfaces of compound semiconductors irradiated with femtosecond laser pulses, Applied Physics Letters 82(25) (2005); Article 4462.

DOI: https://doi.org/10.1063/1.1586457

[10] J. Bonse, S. M. Wiggins and J. Solis, Dynamics of phase transitions induced by femtosecond laser pulse irradiation of indium phosphide, Applied Physics A 80(2) (2005), 243-248.

DOI: https://doi.org/10.1007/s00339-004-3025-z

[11] K. V. Shalimova, Physics of Semiconductors, Energoatomizdat, Moscow, 1985.

[12] Yu. D. Sokolov, About the definition of dynamic forces in the mine lifting, Applied Mechanics 1(1) (1955), 23-35.

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