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RESEARCH ARTICLE

ON APPROACH TO ESTIMATE SPEED OF GROWTH OF FILMS DURING MAGNETRON SPUTTERING

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ABSTRACT

In this paper we analyzed mass transfer during the growth of epitaxial layers in magnetrons. We also estimate growth velocity of the epitaxial layers and analyzed its value as a function of various parameters.
Keywords: mass transfer; magnetrons sputtering; analytical approach for modeling, estimation of growth velocity.

INTRODUCTION

Development of solid-state electronics and widespread using of heterostructures for manufacturing of electronic devices leads to the necessity to improve properties of layers of these heterostructures. Different methods are used to manufacture of heterostructures: molecular beam epitaxy, epitaxy from the gas phase, magnetron sputtering. A large number of experimental works have been devoted to the manufacturing and using of heterostructures due to their widespread using [1-12]. At the same time, a relatively small number of works are devoted to predicting the growth of heterostructures [11, 12].

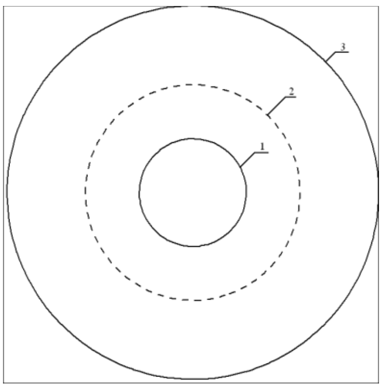

Fig 1: Structure of magnetron. In the framework of the structure ions have been emitted from cathode (line 1). After that under influence of field between cathode (line 1) and anode (line 3) one can obtained flow of ions between lines 1 and 2

In this paper in development of references [13-16] we analyzed processes framework growing films by magnetron sputtering. Structure of the considered magnetron is shown in Fig. 1. Framework the structure electrons are emitting from the cathode (line 1). After that under the action of a field between the cathode (line 1) and the anode (line 3) an electron flow is formed between lines 1 and 2. The main purpose of this work is to analyze the mass transfer in the magnetron during the growth of films in order to improve their properties. To solve this aim an analytical approach for analysis of mass transfer was developed, which makes it possible to take into account the nonlinearity of mass transfer, as well as the changing of its parameters in space and time.

Method of solution

To solve our aims we determine spatio-temporal distribution of electromagnetic field. We determine the distribution by solving the following boundary problem [17, 18]

$$rot\,\vec{H}(r,\varphi,z,t)=\vec{j}+\frac{\partial\vec{D}(r,\varphi,z,t)}{\partial t},\quad rot\,\vec{E}(r,\varphi,z,t)=-\frac{\partial\vec{B}(r,\varphi,z,t)}{\partial t},$$
$$div\,\vec{D}(r,\varphi,z,t)=\rho,\quad div\,\vec{B}(r,\varphi,z,t)=0,\quad \vec{D}=\varepsilon_0\varepsilon\,\vec{E},\quad \vec{B}=\mu_0\mu\,\vec{H}. \tag{1}$$

Here ε and μ are the dielectric and magnetic constants, $\varepsilon_0=0.886\cdot10^{-11}$ F/m, $\mu_0=1.256\cdot10^{-6}$ H/m, $\vec{E}$ and $\vec{H}$ are the electric and magnetic strengths, $\vec{D}$ and $\vec{B}$ are the inductions of electric and magnetic fields. Boundary and initial conditions for the system of equations could be written as

$$B_z(R,\varphi,z,t)=0,\quad D_r(R,\varphi,z,t)=0,\quad E_z(R,\varphi,z,t)=0,\quad H_r(R,\varphi,z,t)=0,$$
$$\vec{E}(r,\varphi,z,0)=\vec{E}_0,\quad \vec{H}(r,\varphi,z,0)=\vec{H}_0.$$

Current density $\vec{j}$ is proportional to speed of ions $\vec{v}$: $\vec{j}=C\cdot\vec{v}$, where C is the density of ions. The speed of ions correlated with strengths of electric and magnetic field by the second Newton law

$$m\frac{d\vec{v}}{dt}=e\left(\vec{E}+\vec{v}\times\vec{B}\right). \tag{3}$$

Scalar form of the Eqs.(1) could be written as

$$C\,v_r+\frac{\partial D_r(r,\varphi,z,t)}{\partial t}=\frac{1}{r}\frac{\partial H_z(r,\varphi,z,t)}{\partial\varphi}-\frac{\partial H_\varphi(r,\varphi,z,t)}{\partial z},$$
$$C\,v_\varphi+\frac{\partial D_\varphi(r,\varphi,z,t)}{\partial t}=\frac{1}{r}\frac{\partial H_z(r,\varphi,z,t)}{\partial\varphi}-\frac{\partial H_r(r,\varphi,z,t)}{\partial z},$$
$$C\,v_z+r\frac{\partial D_z(r,\varphi,z,t)}{\partial t}=\frac{\partial\left[r\,H_\varphi(r,\varphi,z,t)\right]}{\partial r}-\frac{\partial H_r(r,\varphi,z,t)}{\partial\varphi},$$
$$\frac{\partial E_\varphi(r,\varphi,z,t)}{\partial z}-\frac{1}{r}\frac{\partial E_z(r,\varphi,z,t)}{\partial\varphi}=\frac{\partial B_r(r,\varphi,z,t)}{\partial t},$$
$$\frac{\partial E_r(r,\varphi,z,t)}{\partial z}-\frac{1}{r}\frac{\partial E_z(r,\varphi,z,t)}{\partial\varphi}=\frac{\partial B_\varphi(r,\varphi,z,t)}{\partial t},$$
$$\frac{\partial\left[r\,E_\varphi(r,\varphi,z,t)\right]}{\partial r}-\frac{\partial E_r(r,\varphi,z,t)}{\partial\varphi}=r\frac{\partial B_z(r,\varphi,z,t)}{\partial t},$$

$$\frac{1}{r}\frac{\partial\left[r\,D_r(r,\varphi,z,t)\right]}{\partial r}+\frac{1}{r}\frac{\partial D_\varphi(r,\varphi,z,t)}{\partial\varphi}+\frac{\partial D_z(r,\varphi,z,t)}{\partial z}=\rho,$$

$$\frac{1}{r}\frac{\partial\left[r\,B_r(r,\varphi,z,t)\right]}{\partial r}+\frac{1}{r}\frac{\partial B_\varphi(r,\varphi,z,t)}{\partial\varphi}+\frac{\partial B_z(r,\varphi,z,t)}{\partial z}=0,$$

$$m\frac{d\,v_r}{d\,t}=e\left(E_r+v_\varphi B_z\right),\quad m\frac{d\,v_\varphi}{d\,t}=e\left(E_\varphi+v_r B_z\right),\quad m\frac{d\,v_z}{d\,t}=e\left(E_z+v_r B_\varphi\right).$$

To solve these equations we use the method of averaging functional corrections [19]. To determine the first-order approximations of the required functions we replace them in the right-hand sides of equations (4) by their not yet known average values α_{1s} in the right-hand side of these equations. As a result of this substitution we obtain the following equations to determine the first-order approximations of components of strength and induction of the considered fields

$$C\,v_r+\frac{\partial D_{1r}(r,\varphi,z,t)}{\partial t}=0,\quad C\,v_\varphi+\frac{\partial D_{1\varphi}(r,\varphi,z,t)}{\partial t}=0,\quad C\,v_z+\frac{\partial D_{1z}(r,\varphi,z,t)}{\partial t}=\alpha_{1H_\varphi},$$

$$\frac{\partial B_{1r}(r,\varphi,z,t)}{\partial t}=0,\quad \frac{\partial B_{1\varphi}(r,\varphi,z,t)}{\partial t}=0,\quad \frac{\partial B_{1z}(r,\varphi,z,t)}{\partial t}=\alpha_{1E_\varphi},\quad \frac{1}{r}\frac{\partial\left[r\,D_{1r}(r,\varphi,z,t)\right]}{\partial r}=C,$$

$$\frac{1}{r}\frac{\partial\left[r\,B_{1r}(r,\varphi,z,t)\right]}{\partial r}=0,\quad m\frac{d\,v_{1r}}{d\,t}=e\left(\alpha_{1E_r}+\alpha_{1v_\varphi}\alpha_{1B_z}\right),\quad m\frac{d\,v_{1\varphi}}{d\,t}=e\left(\alpha_{1E_\varphi}+\alpha_{1v_r}\alpha_{1B_z}\right),$$

$$m\frac{d\,v_{1z}}{d\,t}=e\left(\alpha_{1E_z}+\alpha_{1v_r}\alpha_{1B_\varphi}\right).$$

Further after integration of left and right sides of these equations on considered variables we obtain the first-order approximations of the considered fields and velocity of ions in the following form

$$D_{1r}(r,\varphi,z,t)=-\int_0^t C\,v_{1r}\,d\,\tau,\quad D_{1\varphi}(r,\varphi,z,t)=-\int_0^t C\,v_{1\varphi}\,d\,\tau,$$

$$D_{1z}(r,\varphi,z,t)=\alpha_{1H_\varphi}t-\int_0^t C\,v_{1z}\,d\,\tau+\varepsilon\,\varepsilon_0 E_0,\quad m v_{1r}=e\left(\alpha_{1E_r}+\alpha_{1v_\varphi}\alpha_{1B_z}\right)t,$$

$$B_{1r}(r,\varphi,z,t)=0,\quad B_{1\varphi}(r,\varphi,z,t)=\mu\,\mu_0 H_0,\quad B_{1z}(r,\varphi,z,t)=\alpha_{1E_\varphi}t,$$

$$m v_{1\varphi}=e\left(\alpha_{1E_\varphi}+\alpha_{1v_r}\alpha_{1B_z}\right)t+m v_{\varphi 0},\quad m v_{1z}=e\left(\alpha_{1E_z}+\alpha_{1v_r}\alpha_{1B_\varphi}\right)t+m v_{z0}.$$

Calculation of average values α_{1s} by using the following standard relation [19]

$$\alpha_{1s_q}=\frac{1}{2\pi\Theta LR^2}\int_0^\Theta\int_0^L\int_0^R r\int_0^{2\pi} S_{1q}(r,\varphi,z,t)\,d\,\varphi\,d\,r\,d\,z\,d\,t$$

(Θ is the continuance of growth, L is the length of magnetron) gives a possibility to obtain, that $\alpha_{1v_z}=v_{z0}+e\Theta^2\left(H_0\Theta^2-\alpha_{1v_z}C\,\Theta^2+4\varepsilon\,\varepsilon_0 E_0\right)/4m$, $\alpha_{1E_\varphi}=0$, $\alpha_{1H_\varphi}=H_0$, $\alpha_{1E_z}=2\varepsilon\,\varepsilon_0 E_0+\Theta^2\left(H_0-\alpha_{1v_z}C\right)/2$, $\alpha_{1E_r}=0$, $\alpha_{1v_r}=0$, $\alpha_{1v_\varphi}=v_{\varphi 0}$.

Further we obtain the second-order approximations of components of strength and induction of electrical and magnetic fields. To obtain these approximations we replace considered fields in right sides of Eqs.

(4) on the following sums $S\,(r,\varphi,z,t)\rightarrow\alpha_{2s}+S_1(r,\varphi,z,t)$. The replacement leads to transformation of Eqs. (4) to the following form

$$C v_{2r} + \frac{\partial D_{2r}(r,\varphi,z,t)}{\partial t} = \frac{1}{r}\frac{\partial H_{1z}(r,\varphi,z,t)}{\partial \varphi} - \frac{\partial H_{1\varphi}(r,\varphi,z,t)}{\partial z},$$

$$C v_{2\varphi} + \frac{\partial D_{2\varphi}(r,\varphi,z,t)}{\partial t} = \frac{1}{r}\frac{\partial H_{1z}(r,\varphi,z,t)}{\partial \varphi} - \frac{\partial H_{1r}(r,\varphi,z,t)}{\partial z},$$

$$C v_{2z} + r\frac{\partial D_{2z}(r,\varphi,z,t)}{\partial t} = \alpha_{2H_\varphi} + H_{1\varphi}(r,\varphi,z,t) + r\frac{\partial H_{1\varphi}(r,\varphi,z,t)}{\partial r} - \frac{\partial H_{1r}(r,\varphi,z,t)}{\partial \varphi},$$

$$\frac{\partial B_{2r}(r,\varphi,z,t)}{\partial t} = \frac{\partial E_{1\varphi}(r,\varphi,z,t)}{\partial z} - \frac{1}{r}\frac{\partial E_{1z}(r,\varphi,z,t)}{\partial \varphi},$$

$$\frac{\partial B_{2\varphi}(r,\varphi,z,t)}{\partial t} = \frac{\partial E_{1r}(r,\varphi,z,t)}{\partial z} - \frac{1}{r}\frac{\partial E_{1z}(r,\varphi,z,t)}{\partial \varphi},$$

$$r\frac{\partial B_{2z}(r,\varphi,z,t)}{\partial t} = \alpha_{2E_\varphi} + E_{1\varphi}(r,\varphi,z,t) + r\frac{\partial E_{1\varphi}(r,\varphi,z,t)}{\partial r} - \frac{\partial E_{1r}(r,\varphi,z,t)}{\partial \varphi},$$

$$\frac{1}{r}\frac{\partial\left[r D_{2r}(r,\varphi,z,t)\right]}{\partial r} = \rho - \frac{1}{r}\frac{\partial D_{1\varphi}(r,\varphi,z,t)}{\partial \varphi} - \frac{\partial D_{1z}(r,\varphi,z,t)}{\partial z},$$

$$\frac{1}{r}\frac{\partial\left[r B_{2r}(r,\varphi,z,t)\right]}{\partial r} = -\frac{1}{r}\frac{\partial B_{1\varphi}(r,\varphi,z,t)}{\partial \varphi} - \frac{\partial B_{1z}(r,\varphi,z,t)}{\partial z},$$

$$m\frac{d v_{2r}}{d t} = e\left\{\alpha_{2E_r} + E_{1r}(r,\varphi,z,t) + \left[\alpha_{2v_\varphi} + v_{1\varphi}(r,\varphi,z,t)\right]\left[\alpha_{2B_z} + B_{1z}(r,\varphi,z,t)\right]\right\},$$

$$m\frac{d v_{2\varphi}}{d t} = e\left\{\alpha_{2E_\varphi} + E_{1\varphi}(r,\varphi,z,t) + \left[\alpha_{2v_r} + v_{1r}(r,\varphi,z,t)\right]\left[\alpha_{2B_z} + B_{1z}(r,\varphi,z,t)\right]\right\},$$

$$m\frac{d v_{2z}}{d t} = e\left\{\alpha_{2E_z} + E_{1z}(r,\varphi,z,t) + \left[\alpha_{2v_r} + v_{1r}(r,\varphi,z,t)\right]\left[\alpha_{2B_\varphi} + B_{1\varphi}(r,\varphi,z,t)\right]\right\}.$$

Integration of left and right sides of the above equations on considered variations gives a possibility to obtain the second-order approximations of the considered fields in the following forms

$$D_{2r}(r,\varphi,z,t) = \frac{1}{r}\frac{\partial}{\partial \varphi}\int_0^t H_{1z}(r,\varphi,z,\tau)\,d\tau - \frac{\partial}{\partial z}\int_0^t H_{1\varphi}(r,\varphi,z,\tau)\,d\tau - \int_0^t C v_{2r}\,d\tau,$$

$$D_{2\varphi}(r,\varphi,z,t) = \frac{1}{r}\frac{\partial}{\partial \varphi}\int_0^t H_{1z}(r,\varphi,z,\tau)\,d\tau - \frac{\partial}{\partial z}\int_0^t H_{1r}(r,\varphi,z,\tau)\,d\tau - \int_0^t C v_{2\varphi}\,d\tau,$$

$$r D_{2z}(r,\varphi,z,t) = \alpha_{2H_\varphi} t + \int_0^t H_{1\varphi}(r,\varphi,z,\tau)\,d\tau + r\frac{\partial}{\partial r}\int_0^t H_{1\varphi}(r,\varphi,z,\tau)\,d\tau - \frac{\partial}{\partial \varphi}\int_0^t H_{1r}(r,\varphi,z,\tau)\,d\tau - $$
$$- C\int_0^t v_{2z}\,d\tau + r\,\varepsilon\,\varepsilon_0 E_0,\quad B_{2r}(r,\varphi,z,t) = \frac{\partial}{\partial z}\int_0^t E_{1\varphi}(r,\varphi,z,\tau)\,d\tau - \frac{1}{r}\frac{\partial}{\partial \varphi}\int_0^t E_{1z}(r,\varphi,z,\tau)\,d\tau,$$

$$B_{2\varphi}(r,\varphi,z,t) = \frac{\partial}{\partial z}\int_0^t E_{1r}(r,\varphi,z,\tau)\,d\tau - \frac{1}{r}\frac{\partial}{\partial \varphi}\int_0^t E_{1z}(r,\varphi,z,\tau)\,d\tau + \mu\,\mu_0 H_0,$$

$$r\,B_{2z}(r,\varphi,z,t)=\alpha_{2E_\varphi}t+\int_0^t E_{1\varphi}(r,\varphi,z,\tau)\,d\tau+r\frac{\partial}{\partial r}\int_0^t E_{1\varphi}(r,\varphi,z,\tau)\,d\tau-\frac{\partial}{\partial\varphi}\int_0^t E_{1r}(r,\varphi,z,\tau)\,d\tau,$$

$$r\,D_{2r}(r,\varphi,z,t)=C\frac{r^2}{2}-\frac{\partial}{\partial\varphi}\int_0^r D_{1\varphi}(u,\varphi,z,t)\,du-\frac{\partial}{\partial z}\int_0^r u\,D_{1z}(u,\varphi,z,t)\,du,$$

$$r\,B_{2r}(r,\varphi,z,t)=-\frac{\partial}{\partial\varphi}\int_0^r B_{1\varphi}(u,\varphi,z,t)\,du-\frac{\partial}{\partial z}\int_0^r u\,B_{1z}(u,\varphi,z,t)\,du,$$

$$m v_{2r}=e\Bigg[\alpha_{2E_r}t+\int_0^t E_{1r}(r,\varphi,z,\tau)\,d\tau+\alpha_{2v_\varphi}\alpha_{2B_z}t+\alpha_{2v_\varphi}\int_0^t B_{1z}(r,\varphi,z,\tau)\,d\tau+$$
$$+\alpha_{2B_z}\int_0^t v_{1\varphi}(r,\varphi,z,\tau)\,d\tau+\int_0^t v_{1\varphi}(r,\varphi,z,\tau)B_{1z}(r,\varphi,z,\tau)\,d\tau\Bigg],$$

$$m v_{2\varphi}=e\Bigg[\alpha_{2E_\varphi}t+\int_0^t E_{1\varphi}(r,\varphi,z,\tau)\,d\tau+\alpha_{2v_r}\alpha_{2B_z}t+\alpha_{2v_r}\int_0^t B_{1z}(r,\varphi,z,\tau)\,d\tau+$$
$$+\alpha_{2B_z}\int_0^t v_{1r}(r,\varphi,z,\tau)\,d\tau+\int_0^t v_{1r}(r,\varphi,z,\tau)B_{1z}(r,\varphi,z,\tau)\,d\tau\Bigg],$$

$$m v_{2z}=e\Bigg[\alpha_{2E_z}t+\int_0^t E_{1z}(r,\varphi,z,\tau)\,d\tau+\alpha_{2v_r}\alpha_{2B_\varphi}t+\alpha_{2v_r}\int_0^t B_{1\varphi}(r,\varphi,z,\tau)\,d\tau+$$
$$+\alpha_{2B_\varphi}\int_0^t v_{1r}(r,\varphi,z,\tau)\,d\tau+\int_0^t v_{1r}(r,\varphi,z,\tau)B_{1\varphi}(r,\varphi,z,\tau)\,d\tau\Bigg].$$

Average values of the second-order approximations α_{2s} were calculated by using the following standard relation [19]

$$\alpha_{2s_q}=\frac{1}{2\pi\Theta LR^2}\int_0^\Theta\int_0^L\int_0^R r\int_0^{2\pi}\left[S_{2q}(r,\varphi,z,t)-S_{1q}(r,\varphi,z,t)\right]d\varphi\,dr\,dz\,dt\,. \tag{5}$$

Substitution of obtained approximations of strength and induction of considered fields and velocities of movement of ions into relations (5) gives a possibility to obtain relations for the required average values in the following form

$$\alpha_{2D_z}=\left(\alpha_{2H_\varphi}-\alpha_{1H_\varphi}\right)\frac{\Theta^2}{6}+\int_0^\Theta\frac{\Theta-t}{2\pi\Theta LR^2}\int_0^L\int_0^R\int_0^{2\pi}H_{1\varphi}(r,\varphi,z,t)\,d\varphi\,dr\,dz\,dt+$$
$$+\int_0^\Theta\frac{\rho(\Theta-t)}{2\pi\Theta LR^2}\int_0^L\int_0^R\int_0^{2\pi}\left(v_{2z}-v_{1z}\right)d\varphi\,dr\,dz\,dt,\quad \alpha_{2D_r}=0,\quad \alpha_{2D_\varphi}=0,\quad \alpha_{2B_z}=0,\quad \alpha_{2B_r}=0,$$
$$\alpha_{2B_\varphi}=\mu\mu_0 H_0,\quad \alpha_{2v_r}=0,\quad \alpha_{2v_\varphi}=-v_{\varphi 0},$$
$$\alpha_{2v_z}=\frac{e}{m}\int_0^\Theta\frac{\Theta-t}{2\pi\Theta LR^2}\int_0^L\int_0^R r\int_0^{2\pi}E_{1z}(r,\varphi,z,t)\,d\varphi\,dr\,dz\,dt-\Theta\frac{e\alpha_{1E_z}}{2m}-v_{z0}.$$

In this paper we calculated the second-order approximations of the required strengths and inductions of the considerate fields, as well as the ion velocities by the method of averaging functional corrections. The approximation is usually sufficient to obtain qualitative conclusions and to obtain some quantitative results. The obtained analytical results were checked by comparing them with the results of numerical simulation.

RESULT

In this section we estimate velocity of growth of epitaxial layers by using the following relation [20]

$$V = \frac{Y\, j\,(r) A}{N_A e C (1+\gamma)}, \tag{6}$$

where $N_A \approx 6.022 \times 10^{23}$ mol^{-1} is the Avagadro number; A is the atomic mass of material, which is sputtering in the considered magnetron; Y is the coefficient sputtering of atomic ions of the sputtering material; j (r) is the discharge current density at the radius r; γ is the coefficient of ion-electron emission of material of the considered target. The Fig. 2 shows dependence of velocity of growth of sputtering material on cyclotron frequency ω_c. Increasing of induction of magnetic field B_0 leads to increasing of the cyclotron frequency ω_c and to increase homogeneity of epitaxial layer and decreasing of velocity of growth. The Fig. 3 shows dependence of velocity of growth of sputtering material on electric strengths E_0. Increasing of the strengths leads to increasing of speed of transport of ions to target and appropriate velocity of growth. In this case the opposite effect was obtained with increasing of the ion mass (see Fig. 3), radius (see Fig. 4) and length (see Fig. 5) of the magnetron.

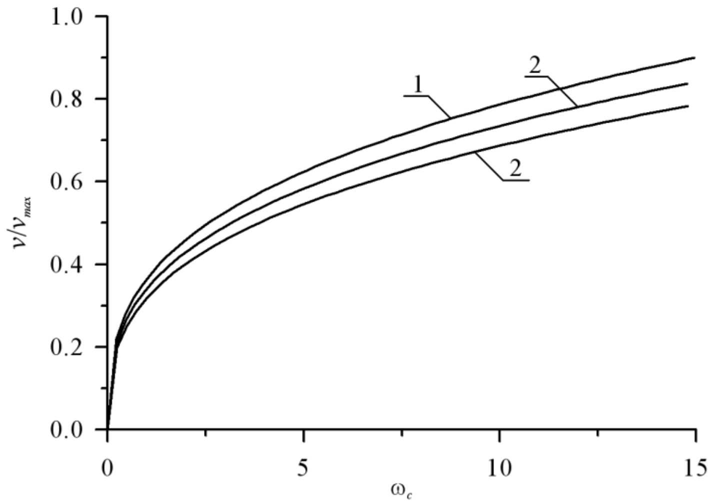

Fig 2: Typical dependence of velocity of growth of sputtered material on cyclotron frequency ω_c. Increasing of density of curves correspond to increasing of strength of electrical field

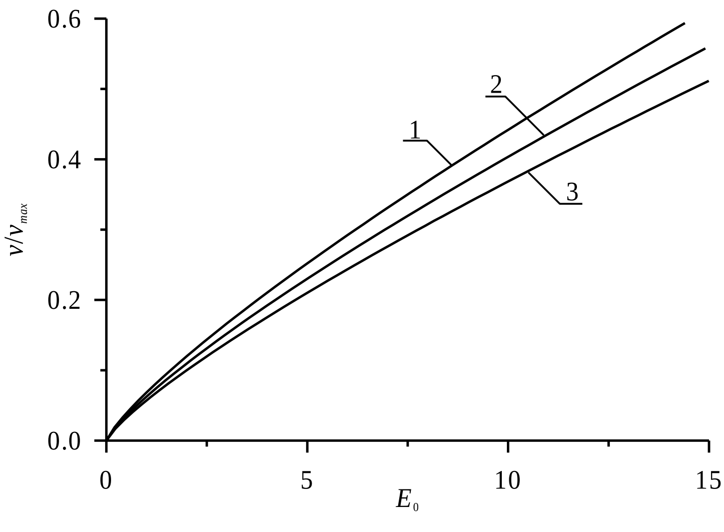

Fig 3: Typical dependence of velocity of growth of sputtered material on electric strengths E_0. Increasing of density of curves correspond to increasing of mass of ions

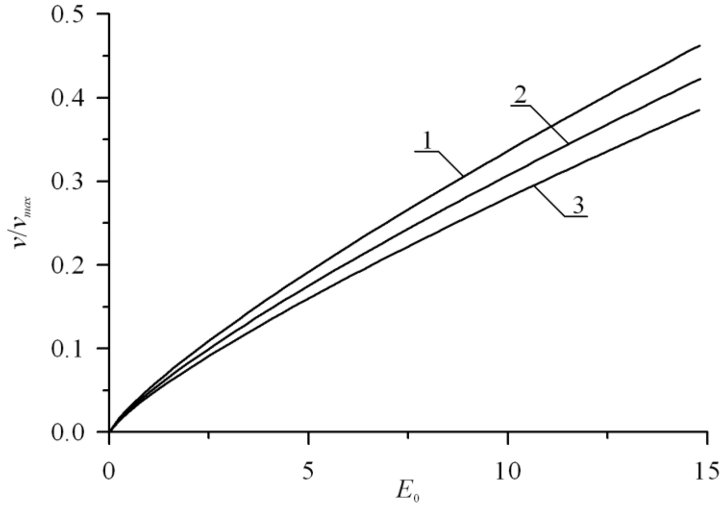

Fig 4: Typical dependence of velocity of growth of sputtered material on electric strengths E_0. Increasing of density of curves correspond to increasing of radius of magnetron

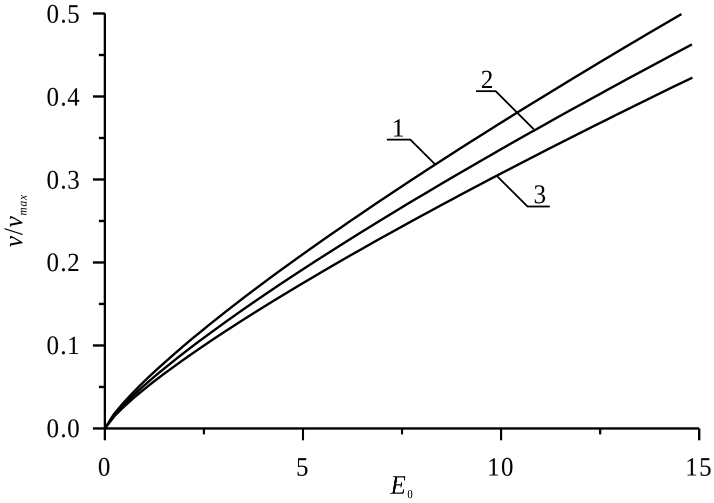

Fig 5: Typical dependence of velocity of growth of sputtered material on electric strengths E_0. Increasing of density of curves correspond to increasing of length of magnetron

CONCLUSION

In the present paper we analyzed mass transport during magnetron sputtering of materials. Based on results of analysis we formulate recommendations to control of velocity of growth of epitaxial layers. We also introduce an analytical approach for prognosis of mass transport during growth of layers in magnetron.

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