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Thermal field of deposited coverings

In work formation of ionic-plasma coverings when film growth is defined by conditions on mobile border of section of phases is considered. The analytical decision of the general problem with any boundary conditions is received. For homogeneous boundary conditions which are closest to technology of drawing of ionic-plasma coverings, the formula for a temperature field of deposited coverings is received. The carried out analysis has shown, that at formation of an ionic-plasma covering there is a wave structure. Comparison with results of measurement of microhardness of a covering along the sample has proved theoretical model. The received result can be used for perfection of technology of drawing of ionic-plasma coverings of a various functional purpose.

Key words: plasma, covering, thermal field, mobile border of section of phases, wave structure, microhardness.

Introduction

One of ways of improvement of properties of a surface of materials is drawing of composite coverings by a method of vacuum ionic-plasma sedimentation [1, 2]. Reception of nanocomposites by means of ionic-plasma methods demands sedimentation on a substrate of multicomponent streams. In most cases synthesis of coverings of difficult element structure is realised by level-by-level or simultaneous sedimentation on a substrate in atmosphere of reactionary gases of streams from two sources: ionic [3], magnetron [4], vacuum-arc [5] and their combinations [6].

Though ways of reception of nanostructural materials and coverings are various enough [7], but all of them are based on the mechanism intensive dissipation the energy generalised in three stages of formation. At the first stage there is a process of formation of germs which in the absence of corresponding thermodynamic conditions, does not pass in mass crystallisation. The second stage represents formation round nanocrystal germs of amorphous clusters which — at the third stage — unite in an intercrystal phase with formation of dissipation structures.

In the present work we will consider the third stage of formation of a covering when film growth is defined by conditions on mobile border of section of phases. Such problems have received the name — a Stefan's problem [8]. From the mathematical point of view regional problems of such type are essentially distinct from classical problems [8, 9]. Owing to dependence of the size of area of carrying over of a stream on time to this type of problems classical methods of division of variable and Furie's integrated transformations as, remaining within the limits of classical methods of mathematical physics, it is not possible to co-ordinate the decision of the equation with movement of border of section of phases are inapplicable. The review of modern achievements in the solution of Stefan's problem is given in the monography [10].

The general statement of a problem

We will consider a problem about crystallisation of a deposited covering on a round substrate, that is a problem about crystallisation of the final cylinder with mobile border of section of phases. The non-stationary equation of heat conductivity describing process of crystallisation in mobile cylindrical system of co-ordinates, moving under the law β(*t*), looks like:

$$\frac{\partial T}{\partial t} = a\left[\frac{\partial^2 T}{\partial z^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)\right], \qquad (1)$$

where *a* — thermal conductivity.

Initial and boundary conditions we will choose in a general view:

$$T(r, z, t)|_{t=0} = \varphi(r, z), \qquad (2)$$

$$T(r, z, t)|_{r=R} = \gamma(z, t), \qquad (3)$$

$$T\left(r,z,t\right)\big|_{z=0}=\gamma_1\left(r,t\right), \tag{4}$$

$$T\left(r,z,t\right)\big|_{z=\beta(t)}=\gamma_2\left(r,t\right). \tag{5}$$

Functions $\beta(t), \varphi(r,z), \gamma(z,t), \gamma_1(r,t)\, u\, \gamma_2(r,t)$ we will consider continuous. For the problem solution we search in a kind:

$$T\left(r,z,t\right)=\sum_{k=o}^{\infty}\bar{T}\left(z,t\right)I_0\left(\lambda_{0k}r\right), \tag{6}$$

where λ_{ok} — equation roots

$$I_0\left(\lambda_{ok}R\right)=0 \tag{7}$$

and $I_0\left(\lambda_{ok}R\right)$ — Bessel's function of the zero order, satisfying to the equation:

$$\frac{1}{r}\frac{d}{dr}\left[r\frac{dI\left(\lambda_{0k}r\right)}{dr}\right]+I_0\left(\lambda_{0k}r\right)=0, \tag{8}$$

$$\bar{T}_k\left(z,t\right)=\int_0^R T_k\left(r,z,t\right)I_0\left(\lambda_0 r\right)rdr. \tag{9}$$

Applying transformation (9) and considering (6) and (7), the equation (1) we will lead to a kind:

$$\frac{1}{a}\frac{\partial\bar{T}_k}{\partial t}=\frac{\partial^2\bar{T}_k}{\partial z^2}+\bar{\Phi}_k\left(z,t\right)-\bar{T}_k\left(z,t\right). \tag{10}$$

Using replacement $\bar{T}_k=\tilde{T}e^{-at}$ and having transformed similarly boundary conditions, we will receive the following problem:

$$\frac{1}{a}\frac{\partial\tilde{T}_k}{\partial t}=\frac{\partial^2\tilde{T}_k}{\partial z^2}+\tilde{\Phi}_{\text{k}}\left(z,t\right), \tag{11}$$

$$\tilde{T}_k\left(z,t\right)\big|_{t=0}=\tilde{\varphi}\left(z\right), \tag{12}$$

$$\tilde{T}_k\left(z,t\right)\big|_{z=0}=\tilde{\gamma}_1\left(t\right), \tag{13}$$

$$\tilde{T}_k\left(z,t\right)\big|_{z=\beta(t)}=\tilde{\gamma}_2\left(t\right), \tag{14}$$

in area $Д:\left(t>0, 0<z<\beta(t)\right)$.

For the solution of a problem (11)–(14) we search in the form of the sum of potentials I and II sorts, and also two potentials of a double layer:

$$\begin{gathered}\tilde{T}_k\left(z,t\right)=\frac{1}{2\sqrt{a}}\int_0^{\ell}\frac{\tilde{\varphi}(\xi)}{\sqrt{\pi t}}e^{-\frac{(z-\xi)^2}{4at}}d\xi+\int_6^t d\tau\int_0^{\ell}\frac{\tilde{\Phi}_k\left(\xi,\tau\right)}{2\sqrt{\pi a\left(t-\tau\right)}}e-\frac{(z-\xi)^2}{4a(t-\tau)}\,d\xi+\\+\frac{1}{4\sqrt{\pi}}\int_0^t\frac{z}{\left[a\left(t-\tau\right)\right]^{3/2}}e^{-\frac{z^2}{4a(t-\tau)}}K_1(\tau)d\tau+\frac{1}{4\sqrt{\pi}}\int_0^t\frac{z-\beta(\tau)}{\left[a\left(t-\tau\right)\right]^{3/2}}e^{-\frac{[z-\beta(\tau)]^2}{4a(t-\tau)}}K_2(\tau)d\tau.\end{gathered} \tag{15}$$

Using conditions (13), (14), we will receive system of the integrated equations:

$$\begin{gathered}\tilde{\gamma}_1'(t)=\frac{K_1(t)}{2a}-\frac{1}{4\sqrt{\pi}}\int_0^t\frac{\beta(\tau)}{\left[a\left(t-\tau\right)\right]^{3/2}}e^{-\frac{\beta^2(\tau)}{4a(t-\tau)}}K_2(\tau)d\tau,\\ \tilde{\gamma}_2'(t)=\frac{K_2(t)}{2a}+\frac{1}{4\sqrt{\pi}}\int_0^t\frac{\beta(t)-\beta(\tau)}{\left[a\left(t-\tau\right)\right]^{3/2}}e^{-\frac{[\beta(t)-\beta(\tau)]^2}{4a(t-\tau)}}K_2(\tau)d\tau+\frac{1}{4\sqrt{\pi}}\int_0^t\frac{\beta(t)}{\left[a\left(t-\tau\right)\right]^{3/2}}e^{-\frac{\beta^2(t)}{4a(t-\tau)}}K_1(\tau)d\tau,\end{gathered} \tag{16}$$

where

$$\tilde{\gamma}_1'(t)=\tilde{\gamma}_1(t)-\frac{1}{2}\int_0^{\ell}\frac{\tilde{\varphi}(\xi)}{\sqrt{\pi at}}e^{-\frac{\xi^2}{4at}}d\xi-\int_0^t d\tau\int_0^{\ell}\frac{\tilde{\Phi}_k(\xi,\tau)}{2\sqrt{\pi a(t-\tau)}}\cdot e^{-\frac{\xi^2}{4a(t-\tau)}}d\xi;$$

$$\tilde{\gamma}_2'(t)=\tilde{\gamma}_2(t)-\frac{1}{2}\int_0^{\ell}\frac{\tilde{\varphi}(\xi)}{\sqrt{\pi at}}e^{-\frac{[\beta(t)-\xi]^2}{4at}}d\xi-\int_0^t d\tau\int_0^{\ell}\frac{\tilde{\Phi}_k(\xi,\tau)}{2\sqrt{\pi a(t-\tau)}}\cdot e^{-\frac{[\beta(t)-\xi]^2}{4a(t-\tau)}}d\xi.$$

Excluding from the first equation of system (16) and substituting in a following equation $K_1(t)$, we have:

$$\tilde{\gamma}_2'(t)=\frac{K_2(t)}{2a}+\frac{1}{4\sqrt{\pi}}\int_0^t \frac{\beta(t)-\beta(\tau)}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{[\beta(t)-\beta(\tau)]^2}{4a(t-\tau)}}K_2(\tau)d\tau+\frac{2a}{\sqrt{\pi}}\int_0^t \frac{\beta(t)}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{\beta^2(t)}{4a(t-\tau)}}\tilde{\gamma}_1'(\tau)d\tau+$$
$$+\frac{a}{8\pi}\int_0^t \frac{\beta(t)}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{\beta^2(t)}{4a(t-\tau)}}\left(\int_0^\tau \frac{\beta(\tau_1)}{a(t-\tau)^{3/2}}e^{-\frac{\beta^2(t)}{4a(t-\tau)}}K_2(\tau_1)d\tau_1\right)d\tau. \qquad (17)$$

Entering a designation

$$q(t)=\tilde{\gamma}_2(t)-\frac{a}{2\sqrt{\pi}}\int_0^t \frac{\beta(t)}{\left[a(t-\tau)\right]^{3/2}}\tilde{\gamma}_1'(\tau)e^{-\frac{\beta^2(t)}{4a(t-\tau)}}d\tau, \qquad (18)$$

and calculating integral in (17), we will receive

$$-\frac{K_2(t)}{2a}+\frac{1}{4\sqrt{\pi}}\int_0^t \frac{\beta(t)-\beta(\tau)}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{[\beta(t)-\beta(\tau)]^2}{4a(t-\tau)}}K_2(\tau)d\tau+\frac{1}{4\sqrt{\pi}}\int_0^t \frac{\beta(t)}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{\beta(t)^2}{4a(t-\tau)}}K_2(\tau)d\tau=q(t). \qquad (19)$$

Designating,

$$\lambda=\frac{1}{2\sqrt{a}},\ f(t)=2aq(t), K(t,\tau)=\frac{\lambda}{\sqrt{\pi}}\frac{\beta(t)-\beta(\tau)}{(t-\tau)^{3/2}}\ e^{-\lambda^2\frac{[\beta(t)-\beta(\tau)]^2}{(t-\tau)}}+\frac{\lambda}{\sqrt{\pi}}\frac{\beta(t)}{(t-\tau)^{3/2}}e^{-\lambda^2\frac{\beta(t)^2}{(t-\tau)}}, \qquad (20)$$

we receive the integrated equation

$$K_2(t)-\int_0^t K(t,\tau)\,K_2(t,\tau)\,d\tau=f(t). \qquad (21)$$

The integrated equation (21) is Voltaire's equation in, $C(0,\ell)$ in only case when, when:

$$\lim_{t\to 0}\int_0^t K(t,\tau)d\tau=0.$$

Really, considering, that $e^{-z}<1$ at, $z>0$ it is easy to show, that the equality resulted above is carried out. Then for the equation (21) there is a unique solution which looks like:

$$K_2(t)=\sum_{n=0}^{\infty}K_{2,n}(t), \qquad (22)$$
$$K_{2,0}(t)=f(t),$$
$$K_{2,1}(t)=\int_0^t K(t,\tau)\,K_{2,0}(\tau)d\tau,$$
$$K_{2,2}(t)=\int_0^t K(t,\tau)\,K_{2,1}(\tau)d\tau,$$
$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$
$$K_{2,n}(t)=\int_0^t K(t,\tau)\,K_{2,n-1}(\tau)d\tau$$
$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$

and a number (22) converges absolutely and in regular intervals in topology $C(0,\ell)$.

Then

$$K_1(t)=2a\tilde{\gamma}_1(t)+\frac{a}{2\sqrt{\pi}}\int_0^t \frac{\beta(t)}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{\beta^2(\tau)}{4a(t-\tau)}}\sum_{n=0}^{\infty}K_{2,n}(\tau)d\tau. \qquad (23)$$

Carrying out return transformation, it is definitively had:

$$T(r,z,t)=\sum_{\kappa=0}^{\infty}J_0(\lambda_{o\kappa}r)\left\{e^{-at}\left[\frac{1}{2a\sqrt{\pi}}\int_0^t e^{\frac{(z-\xi)^2}{4at}}dt\left(\int_0^{\ell}\varphi(r,\xi)I_0(\lambda_{ok}r)rdr\right)d\xi+\frac{RI_1(\lambda_{ok}R)}{2\sqrt{\pi}a}\int_0^t d\tau\int_0^{\ell}\frac{\gamma(\xi,\tau)}{\sqrt{t-\tau}}e^{-at}e^{-\frac{(z-\xi)^2}{4a(t-\tau)}}d\xi+\right.\right.$$

$$\left.\left.+\frac{1}{4\sqrt{\pi}}\int_0^t\frac{z}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{z^2}{4a(t-\tau)}}K_1(\tau)d\tau+\frac{1}{4\sqrt{\pi}}\int_0^t\frac{z-\beta(\tau)}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{[z-\beta(\tau)]^2}{4a(t-\tau)}}K_2(\tau)d\tau\right]\right\}. \qquad (24)$$

Thus, the analytical solution of a problem on crystallisation of the cylinder of the final sizes is received. The equation (24) gives in to the numerical solution under the set initial and boundary conditions (2)–(5).

Homogeneous boundary conditions

Sedimentation of ionic-plasma coverings carry out, as a rule, at constant temperature of a substrate. In this case directed by a problem it is possible to use homogeneous boundary conditions. Then the problem (1)–(5) registers in the following formulation:

$$\frac{\partial T}{\partial t}=a\left[\frac{\partial^2 T}{\partial z^2}+\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right)\right] \qquad (25)$$

$$\left.\begin{aligned}&T(r,z,t)\,|_{t=0}=0;\\&T(r,z,t)\,|_{r=R}=T_0=const;\\&T(r,z,t)\,|_{z=0}=T_0=const;\\&T(r,z,t)\,|_{z=\beta(t)}=T_0=const\end{aligned}\right\}, \qquad (26)$$

where T_0 — value of temperature on a surface of the cylinder and on mobile border of section of environments.

Then the common solution of a problem (24) will become:

$$T(r,z,t)=\sum_{\kappa=0}^{\infty}I_0(\lambda_{o\kappa}r)\left\{e^{-at}\left[\frac{RI_1(\lambda_{o\kappa}R)}{2\sqrt{\pi a}}\int_0^t d\tau\int_0^H\frac{T_0}{\sqrt{t-\tau}}e^{-at}e^{-\frac{(z-\xi)^2}{4a(t-\tau)}}d\xi+\frac{1}{4\sqrt{\pi}}\int_0^t\frac{z}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{z^2}{4a(t-\tau)}}K_1(\tau)d\tau+\right.\right.$$

$$\left.\left.+\frac{1}{4\sqrt{\pi}}\int_0^t\frac{z-\beta(\tau)}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{[z-\beta(\tau)]^2}{4a(t-\tau)}}K_2(\tau)d\tau\right]\right\}. \qquad (27)$$

We need to calculate integrals:

$$I_1=\int_0^t d\tau\int_0^H\frac{T_0}{\sqrt{t-\tau}}e^{-a\tau}e-^{\frac{(z-\xi)^2}{4a(t-\tau)}}\,d\xi, \qquad (28)$$

$$I_2=\int_0^t\frac{z}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{z^2}{4(t-\tau)}}K_1(\tau)d\tau, \qquad (29)$$

$$I_3=\int_0^t\frac{z-\beta(\tau)}{\left[a(t-\tau)\right]^{3/2}}e^{-\frac{[z-\beta(\tau)]^2}{4a(t-\tau)}}K_2(\tau)d\tau. \qquad (30)$$

At big times of sedimentation of a covering t integrals I_2 also I_3 are very small and $e^{-at}\to 1$. Then the problem is reduced to integral calculation I_1:

$$I_1=\int_0^t d\tau\int_0^H\frac{\gamma(\xi,\tau)}{\sqrt{t-\tau}}e^{-a\tau}e^{-\frac{(z-\xi)^2}{4a(t-\tau)}}d\xi=T_0\int_0^t\frac{e^{-a\tau}}{\sqrt{t-\tau}}I_1'(\tau)d\tau. \qquad (31)$$

To calculate $I_1'(\tau)$ in (31) we will make replacement of variables $y=\dfrac{z-\xi}{\sqrt{4a(t-\tau)}}$ then we will receive:

$$I_1'(\tau)=\sqrt{4a(t-\tau)}\left[\int\limits_0^{z_2} e^{-y^2}dy-\int\limits_0^{z_1} e^{-y^2}dy\right], \tag{32}$$

where $z_1=\dfrac{z}{\sqrt{4a(t-\tau)}}$, $z_2=\dfrac{z-H}{\sqrt{4a(t-\tau)}}$.

Integrals in square brackets represent function:

$$erfz=\frac{2}{\sqrt{\pi}}\int\limits_0^{z} e^{-y^2}dy\ . \tag{33}$$

Using the formula (33) and its decomposition abreast, after simple calculations we will receive:

$$I_1'(\tau)=\left[ze^{-\frac{z^2}{\sqrt{4a(t-\tau)}}}-(z-H)e^{-\frac{(z-H)^2}{\sqrt{4a(t-\tau)}}}\right]. \tag{34}$$

Substituting (34) in (31), and calculating, we will receive:

$$I_1=\frac{2\sqrt{a}}{z-H}\cdot T_0\,. \tag{35}$$

Being limited to the first member in the sum (27), for stationary temperature it is had following expression:

$$T(r,z)=\frac{T_0R}{\sqrt{\pi}(z-H)}I_0\left(\frac{2r}{R}\right)+C_1+C_2\,. \tag{36}$$

Here C_1, C_2 — integration constants. At reception (36) we have considered, that from the equation $I_0(\lambda_{ок}r)=0$ follows $\lambda_0=2r/R$ and $I_1(2)=1$.

Comparison with experiment

For the qualitative analysis of the received results and their comparison with experimental data, we will be limited to consideration of the equation (36), lowering integration constants. For quantitative calculations, it is necessary to use all members of some (27) taking into account boundary conditions (26). Also we will consider only radial working out the equations (36), considering a small thickness of a covering. Thus, we will consider function:

$$T(r)=\frac{T_0R}{\sqrt{\pi}h}I_0\left(\frac{2r}{R}\right). \tag{37}$$

The schedule of function (37) is resulted in all textbooks on special functions and represents a fading wave. After crystallisation on a surface of the sample the wavy structure should be formed. Experimentally formation of such structure can be checked up, measuring microhardness up and down the sample as distribution of temperature along a surface of the sample leads to distribution of thermal pressure.

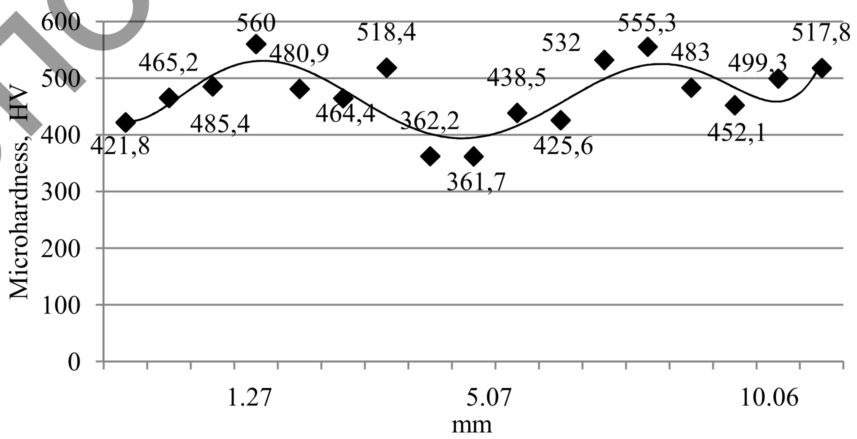

Figure. Microhardness of a covering 12X18H10T + Ti in nitrogen along the sample

The experimental data received by us are shown in Figure. Microhardness measurements were spent at loading of 0,1 kg that corresponds 0,989 N, and time of endurance of loading 15 seconds Similar results are received for the big number of various coverings. The wavy structure is always formed. Measurements were spent concerning the sample without a covering to exclude influence of an initial roughness.

Results of experiment confirm the basic conclusion of the offered theoretical model about formation of wavy structure of an ionic-plasma covering. What practical conclusions it is possible to make of the offered model?

First, formation of wavy structure at covering sedimentation leads to increase in an initial roughness of the sample. It is the fact at drawing of coverings by an ionic-plasma method it is known for a long time already [1]. In this case the big role is played by temperature of sample T_0 at which covering drawing is made. From the equation (37) follows, that the temperature of the sample is necessary for supporting as it is possible more low. However at ionic-plasma drawing of coverings of it to reach not always it is possible. The low temperature of the sample can be supported at magnetron or chemical ways of drawing of coverings. In case of drawing of frictional coverings with the big factor of a friction, formation of wavy structure of a covering is a positive effect.

Secondly, with increase in the size of sample R function $I_0(2r/R)$ decreases more slowly, than increases $T(r)$ at the expense of linear dependence on the size of the sample. The optimum size of the sample is reached under a condition — $I_0(2r/R) = 1/R$.

The conclusion

In case of ionic-plasma coverings process of their formation in a mode of real time is not observed yet owing to specificity of technological process. Therefore the basic information turns out at a variation, both structure of a deposited material, and technological parametres of sedimentation. In this connection the role as computer [11, 12], and analytical models sharply increases.

Numerical methods have received wide application in connection with occurrence of new generation of the computer. These methods are based on replacement of any differential equations with corresponding approximations in final differences. The basic lack of these methods is absence of the approached analytical form of the solution which are often more convenient, than tables and schedules. Besides, presence of the big number of characteristic parametres of a problem and a wide range of their change do results of numerical calculations beloved and inconvenient for their interpretation and practical use.

Despite lacks, numerical methods now play defining role in development of scientific and technical progress, being the device of research of the technical and economic problems connected first of all with planning, optimisation, management and designing of devices and technological processes.

The important advantage of analytical methods is possibility of reception of result of research in the form of the formula allowing simply and visually to track dependence of any property from entry conditions, external influences, parametres of system and its structure.

The problem of analytical research of formation of ionic-plasma coverings is rather difficult at their full description and can be finished only in the elementary cases. Therefore at an analytical method of its solution at once aspire to limit to studying of whenever possible simplified models of system. One of such analytical models also has been considered in the present work.

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Жамылғыны жауып жатқан жылулық өріс

Мақалада иондық-плазмалы жабындының құрылымы қарастырылған, қабыршықтардың өсу шарттары фаза тарауының қозғалғыш шекарасында анықталды. Ортақ мақсаттың талдағыш шешімі өндіргіштік шекаралық шарттармен алынған. Бірыңғай иондық-плазмалы жабындының технологиясына деген ең жақын шекаралық шарттар үшін, жауып жатқан жабындының температуралық өрісі үшін формула алынған. Зерттеу нәтижелері көрсеткендей, иондық-плазмалы жабындының құрылымында толқындық құрылым туады. Жабындының микроқаттылықты өлшеу нәтижелерімен салыстырғандағы үлгі қағидалы қалыптың дұрыстығын растады. Алынған қорытынды әр түрлі функциялық мақсатта иондық-плазмалы жабындының технологиясын жетілдіру үшін пайдаланылуы мүмкін.

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Тепловое поле осаждаемых покрытий

В работе рассмотрено формирование ионно-плазменных покрытий, когда рост пленки определяется условиями на подвижной границе раздела фаз. Получено аналитическое решение общей задачи с произвольными граничными условиями. Для однородных граничных условий, которые наиболее близки к технологии нанесения ионно-плазменных покрытий, получена формула для температурного поля осаждаемых покрытий. Проведенный анализ показал, что при формировании ионно-плазменного покрытия возникает волновая структура. Сравнение с результатами измерения микротвердости покрытия вдоль образца подтвердило правильность теоретической модели. Полученный результат может быть использован для совершенствования технологии нанесения ионно-плазменных покрытий различного функционального назначения.

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