INVESTIGATION OF THERMAL CONDUCTIVITY OF NANOSTRUCTURES USING A MATHEMATICAL MODEL

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Abstract. The transfer of heat through nanostructures differs significantly from the corresponding processes inside macroscopic bodies. Various research methods, both theoretical and experimental, are applied to such objects. This approach to nanostructures gives great advantages. The hyperbolic equations we have obtained describe the wave process of the thermal signal flow and the properties of heat transfer in nanostructures across a thin layer, in which the simplest task is to determine the thermal conductivity.

1. The first section in your paper

The study of nanostructures from the point of view of heat transfer in them is important because of the rapid development of semiconductor lasers that increase radiation properties, and the presence of various structures in almost all fields of science, technology and others.

First of all, dimensional effects that are absent in macroscopic solids attract attention. The dimensional effects can be classical in the range from 1 nm to 100 nm and quantum, which are realized at scales comparable to the de Broglie wavelength.

Active studies of nanostructures have been started relatively recently [1-6], although the statistical theory of thermal conductivity of solids was founded in the works of Peierls and Clemens [7, 8].

Nanostructures (multilayer nanofilms) are artificially formed layered structures consisting of a large number (up to tens of thousands) of alternating nanolayers of various materials. The list of materials used to create multilayer nanostructures is quite wide – it can be pure metals, alloys, semiconductor materials, materials with dielectric properties in various combinations. The thickness of the layers of multilayer nanostructures, as a rule, is in the range from 1 to 100 nm. It is worth noting that the greatest interest is the study of multilayer nanostructures with layers of thickness from units to several tens of nanometers. This is due to the fact that it is in this range that the degree of influence of the dimensional factors of nanolayers on the structure and properties of materials acquires the greatest importance. Thus, the ultra-small thickness of the layers in combination with a large number of interfaces between the layers and the alternation of layers of different materials leads to the appearance of multilayer nanostructures with unique structural features that are not present in the materials that make up the nanostructures in massive samples [9].

A one-dimensional unsteady process of heat propagation in a thermally insulated ordered multilayer nanostructure consisting of several alternating layers of AlAs and GaAs materials is considered.

The heat transfer process (heat signal) occurs in the AlAs layer, and the positive signal simultaneously with the heat flow is the main effect on the GaAs layer. During the pulse, a positive
thermal signal on the surface is subjected to such a dose of energy to realize the decomposition of the upper layer of the material and achieve a voltage of the order of several megabars on the surface. In this case, the pulse goes to the lateral surface covered with AlAs depending on the time.

The mathematical model describing these processes in the simplest isotropic case consists of the energy conservation equation for the subsystem layer and the equation for the relaxation of the heat flow for the subsystem layer.

At the beginning of the process, when the flow of the thermal signal is just beginning to grow, the term with the derivative of the flow is very small, and the traditional approximation works. Therefore, the mathematical model is described in the form of a nonlinear heat equation:

\[
\frac{\partial T}{\partial t} = \frac{k_1 k_2}{k_3 T^{3/2}} \frac{\partial}{\partial x} \left( T^{5/2} \frac{\partial T}{\partial x} \right),
\]

where

\[
k_1 = \frac{k_0 T_0^2 t_0}{\tau_0 P_0}, \quad k_2 = \frac{P_0}{\rho C_t t_0}, \quad k_3 = \frac{t_0}{\tau_0 T_0^{1/2}},
\]

- \( k_1 \) - coefficient of thermal conductivity; \( C_t \) - the heat capacity of the substance; \( \tau_0 \) - relaxation time of the heat flow; \( t \) - time; \( x \) - coordinate; \( T = T(x,t) \) - temperature; \( P_0 \) - maximum flow of the heat signal.

By introducing an integral function

\[
W(T) = \frac{T^{3/2}}{t_0} dT = 2 \left( T^{5/2} - T_0^{5/2} \right)
\]

equation (1) can be reduced to the form:

\[
\frac{\partial W}{\partial t} = \beta \frac{\partial^2 W}{\partial r^2},
\]

where

\[
\beta = \frac{k_1 k_2}{k_3} \left( \frac{m^3 \cdot K}{D_J} \right).
\]

In the low temperature region, the heat transfer process (heat signal) in the AlAs layer decreases sharply with a decrease in temperature, the main effect is on the GaAs layer, as a result of which the free path increases sharply and reaches a value comparable to the size of the GaAs layer. Since the walls of the layer have a low reflection coefficient, a further decrease in temperature does not lead to an increase in the free path length, since in this case it is determined precisely by the size of the GaAs layer. The value of the thermal conductivity coefficient for temperature is small, so the dependence of the thermal conductivity coefficient \( \beta \) on \( W(T) \) will be insignificant. The temperature dependence of the thermal conductivity of the layer in this temperature range is determined by the dependence of the thermal capacity AlAs (GaAs) on temperature. At low temperatures, the heat capacity is proportional to \( T^{5/2} \), and the coefficient of thermal conductivity is also proportional to \( T^{5/2} \).

Given the above, the following assumption will be quite true:

\[
W(T) = W(x,t).
\]

Note that equation (3) with respect to the function \( W(T) \) is linear. Since the coefficient of thermal conductivity \( \lambda(T) = T^{5/2} \) depends on temperature, and the coefficient \( \beta = \frac{k_1 k_2}{k_3} \left( \frac{m^3 \cdot K}{D_J} \right) \) weakly depends on the function \( W(T) \), for an AlAs layer with a low coefficient of thermal conductivity \( T^{5/2} \), the dependence of \( \beta \) on \( W(T) \) can be neglected.
Our goal is to determine the heat transfer in the layered structure at a subsequent time by the method of artificial hyperbolization [1], that is, we will look for a solution to the hyperbolic equation of thermal conductivity:

$$\alpha \frac{\partial^2 W}{\partial t^2} + \frac{\partial W}{\partial t} = \beta \frac{\partial^2 W}{\partial r^2},$$  \hspace{1cm} (4)

where $\alpha$ is the regularization parameter (relaxation time of the heat flow, (ns)).

In the case of a plane geometry, the heat transfer in a layered structure, relative to the function $W(x,t)$ according to [10], has the form:

$$W_0(x,t) = \sum _{k=1}^{\infty } W_{0k} \exp (-\omega _k(\alpha ) t^*)$$

$$\times \left[ 1 + \alpha \frac{\omega _k(\alpha )}{1-4\alpha \beta \eta _k^2} \left( \exp \left( \frac{-\sqrt{1-4\alpha \beta \eta _k^2}}{\alpha } t^* \right) - 1 \right) \right] \sin (\eta _k x).$$  \hspace{1cm} (5)

$$\omega _k(\alpha ) = \frac{2\beta \eta _k^2}{1+\sqrt{1-4\alpha \beta \eta _k^2}}$$

where $\eta _k$ - the coefficient of dielectric permittivity (see [5]).

This relation (2) allows us to find the temperature distribution in nanostructures with a known physical characteristic of materials.

Then

$$T_0(x,t) = \left[ T_{00}(x) \right]^{\frac{1}{2}} + 3.5 W_0(x,t).$$  \hspace{1cm} (6)

The heat flow functions $q_0(x,t)$ and $T_a(x,t)$ are connected in layers as follows:

$$q_0(x,t) = -\left( T_a(x,t) \right)^{\frac{1}{2}} \frac{\partial T_a}{\partial x} x=x_0.$$  \hspace{1cm} (7)

Thus, from the expressions (4) and (6) obtained, it is possible to determine the values of the temperature and heat flux of the substance in the layers. If the temperature and heat flow of the substance are known, the desired thermophysical characteristics (thermal conductivity - $\lambda$, specific heat capacity - $c_p$, density - $\rho$) on the surface of a substance, it can be determined by solving the nonlinear equation (1) in the form of expressions (4) and (6).

In the course of the work, numerical calculations were carried out according to the algorithm constructed according to the regularization scheme in the form of expressions (5) and (6). The study was carried out in a thermally insulated ordered multilayer nanostructure consisting of 400 alternating layers of AlAs and GaAs materials.

As a reference, the thermophysical characteristics of the materials under consideration are given (table 1) [11].

| Thermophysical characteristics | Material | Material |
|-------------------------------|----------|----------|
| C, J/kg*K                    | AlAs     | GaAs     |
| $\rho$, kg/m$^3$             | 424      | 327      |
| $v_s$, m/s                   | 3730     | 5320     |
| $\rho_k$, m2*K/W             | 0,625*10$^{-9}$ | 5242 |

Table 1. Thermophysical characteristics of materials.
The results are presented in the form of graphs (Fig. 1.a) and b)) depending on the material properties of the layers, their thickness and the conductivity of the interfaces between the layers. Figure 1 (a) and 1 (b) show small and large temperature jumps at the boundaries of the layers due to the different magnitude of the singularity.

From the numerical calculation results obtained, it follows that with increasing layer thickness, the phenomenon of heat transfer slows down. So, in multilayer nanostructures, the thickness of the layers has a value of 10-100 nm. The calculation was obtained at different layer thicknesses for the case of the same thickness of the AlAs and GaAs layers. In the calculation, it was also found that the ratio between the heat transfer rates is preserved over time at different layer thicknesses. Therefore, naturally, in the vicinity of the boundary of monotonous instability of the problem with respect to long-wave thermal signals, the equation connecting $k_1$, $k_2$ and $k_3$, using the method of artificial hyperbolization, is a stable calculation for the thermal conductivity of nanostructures.

![Figure 1. a) Characteristic temperature distribution over layers of AlAs and GaAs nanostructure at thickness h=10 nm and time t=1.5*10-6 c; b) results of work [11]](image)
Based on the results obtained and the presented graphic material, it can be said that the stability, the time to enter the mode and the temperature control error of the nanostructure are influenced by the temperature boundary characteristics, the temperature range and the type of material, as well as the regularization parameter (relaxation time). Moreover, it should be noted that each of the above factors has its own degree of influence on the parameters of solving the problem for the nonlinear wave equation of thermal conductivity, and this method of solving by regularization is stable. Low-temperature plasma can be used for the synthesis of various nanostructures and is well suited for the modification of various surfaces. This is shown in many works [12-26].

References
[1] Dmitriev A.S. Thermal processes in nanostructures. -M.: Publishing house of MEI, 2012. -302 p.
[2] Fisher T.S. Thermal Energy at the Nanoscale. - Singapore: World Scientific, 2013. - 171 p.
[3] Cahill D.G., Ford W.K., & Goodson K.E., Madhan G.D., Madjumar A., Maris H.J., Merlin R. Nanoscale Thermal Transport // J. Appl. Phys., 2003, V. 93, № 2. - P. 793-802.
[4] Cahill D.G., Braun P.V., & Chen G., Clarke D.R., Fan S., Goodson K.E., Keblish P., et al. Nanoscale Thermal Transport II. // Appl. Phys. Rev, 2014, V. 1, № 1. - P. 011305. [3]
[5] Dmitriev A.S. Thermal processes in nanostructures. -M.: BINOM, 2015. - 792 p. [3]
[6] Khvesyuk V.I., Scriabin A.S. Thermal conductivity of nanostructures // Thermophysics of High Temperatures, 2017, volume 55, No. 3. - pp. 447-471.
[7] Peierls R.E. Zur kinetischen Theorie der Warmelitung in Kristallen // Ann. Phys. 1929, V. 395. - P. 1055-1066. [3]
[8] Klemens P. Thermal Conductivity and Lattice Vibrational Modes // Solid State Phys., 1958, V. 7. - P. 1-23.
[9] Bazaleeva, K.O. Structure transitions in multilayer nanofilms Ti/Al / K.O. Bazaleeva, V.S. KraPosehin, P.A. Tsygankov et al. // Materials Science. - 2008. - No. 8. - pp. 35-39.
[10] Juraev, H.S. Phenomena of energy and mass transfer in condensed media: mathematical modeling, optimization, practical applications. /H.S. Juraev // Dushanbe: ER-graph. - 2021. - 236 p.
[11] Vorobyov, D.A. Method of calculation of nonstationary heating of nanostructures / D.A. Vorobyov, V.I. Khvesyuk // Science and Education (Electronic Scientific and Technical Journal) of Bauman Moscow State Technical University. 2013. -No.9. -pp.541-550. http://technomag.bmstu.ru/doc/617255.html
[12] Shamsutdinov, R. S., & Timerkaev, B. A. (2021, April). The influence of a supersonic flow of gas at glow discharge. In Journal of Physics: Conference Series (Vol. 1870, No. 1, p. 012019). IOP Publishing. DOI 10.1088/1742-6596/1870/1/012019.
[13] Saifutdinov, A. I., & Sofronitskii, A. O. (2021). Numerical Study of Breakdown and Formation Dynamics of Arc Discharge Plasma Parameters at Ultrahigh Pressures. High Energy Chemistry, 55(3), 228-232.DOI: 10.1134/S0018143921030115
[14] Shemakhin, A. Y., Zheltukhin, V. S., Shemakhin, E. Y., Terentev, T. N., & Sofronitsky, A. O. (2020, July). Experimental installation to study the RF plasma flow at low pressures with experiment data synchronization. In Journal of Physics: Conference Series (Vol. 1588, No. 1, p. 012018). IOP Publishing. DOI: 10.1088/1742-6596/1588/1/012018
[15] Saifutdinova, A. A., Sofronitskii, A. O., Timerkaev, B. A., & Saifutdinov, A. I. (2020). Plasma-Chemical Decomposition of Hydrocarbons on the Basis of the Micro-Arc Discharge with Disc Electrodes Rotating in the Bulk of Raw Materials. Russian Physics Journal, 62(11), 2132-2136.DOI: 10.1007/s11182-020-01957-0
[16] Fairushin, I. I., Saifutdinov, A. I., & Sofronitskiy, A. O. (2020). Numerical and Experimental Studies of the Synthesis of Copper Nanoparticles in a High-Pressure Discharge. High Energy Chemistry, 54(2), 150-153. DOI: 10.1134/S0018143920020071
[17] Asadullin, T. Y., Galeev, I. G., Sofronitskiy, A. O., & Gizeev, M. M. (2019, November). Acoustic impact on electric discharge parameters during sterilization of freeze-dried products. In Journal of Physics: Conference Series (Vol. 1370, No. 1, p. 012016). IOP Publishing. DOI: 10.1088/1742-6596/1370/1/012016

[18] Fairushin, I. I., Saifutdinov, A. I., Sofronitskiy, A. O., Timerkaev, B. A., & Dautov, G. Y. (2019, October). Development of plasma reactor design for synthesis of copper nanoparticles using multi-scale simulation. In Journal of Physics: Conference Series (Vol. 1328, No. 1, p. 012088). IOP Publishing. DOI: 10.1088/1742-6596/1328/1/012088

[19] Asadullin, T. Y., Galeev, I. G., & Sofronitskiy, A. O. (2019, October). The application of pulsed discharge for sterilization of freeze-dried product. In Journal of Physics: Conference Series (Vol. 1328, No. 1, p. 012071). IOP Publishing. DOI: 10.1088/1742-6596/1328/1/012071

[20] Timerkaev, B. A., Ganieva, G. R., Kaleeva, A. A., Israfilov, Z. K., & Sofronitskii, A. O. (2019). Growing of carbon nanotubes from hydrocarbons in an arc plasma. Journal of Engineering Physics and Thermophysics, 92(5), 1248-1252. DOI: 10.1007/s10891-019-02040-3

[21] Dautov, G. Y., Kashapov, N. F., Dautov, I. G., & Sofronitskiy, A. O. (2018, July). Research of the influence of the geometry of the discharge chamber on the characteristics of the arc plasmatron. In Journal of Physics: Conference Series (Vol. 1058, No. 1). IOP Publishing. DOI: 10.1088/1742-6596/1058/1/012035

[22] Timerkaev, B. A., Andreeva, A. A., & Sofronitskiy, A. O. (2017, November). Discharge creeping along the surface in the process for producing nanomaterials. In Journal of Physics: Conference Series (Vol. 927, No. 1, p. 012069). IOP Publishing. DOI: 10.1088/1742-6596/927/1/012069

[23] Sadikov, K. G., Sofronitskiy, A. O., & Larionov, V. M. (2017, November). The effect of electrically conductive additives on the plasma pyrolysis of heavy hydrocarbons. In Journal of Physics: Conference Series (Vol. 927, No. 1, p. 012046). IOP Publishing. DOI: 10.1088/1742-6596/927/1/012046

[24] Timerkaev, B. A., Andreeva, A. A., & Sofronitskiy, A. O. (2017). Discharge creeping along the surface in the process of cleaning and strengthening of the materials surface. In Journal of Physics: Conference Series (Vol. 789, No. 1). IOP Publishing. DOI: 10.1088/1742-6596/789/1/012063

[25] Sadikov, K. G., Sofronitskiy, A. O., & Dautov, I. G. (2017). Functional plasma sprayed coatings on magnesium ceramic substrates. In Journal of Physics: Conference Series (Vol. 789, No. 1, p. 012043). IOP Publishing. DOI: 10.1088/1742-6596/789/1/012043

[26] Timerkaev, B. A., Sofronitskiy, A. O., & Andreeva, A. A. (2016). Carbon nanotubes formation in the decomposition of heavy hydrocarbons creeping along the surface of the glow discharge. In Journal of Physics: Conference Series (Vol. 669, No. 1, p. 012062). IOP Publishing. DOI: 10.1088/1742-6596/669/1/012062