Peculiarities of determining the effective thermal conductivity of multilayer nanostructures under unsteady heating

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Abstract. Some features of pulse heating method are considered to study the main regularities of changes in the temperature of thin films in application to flash method. Heat exchange with the surrounding space is taken into account. The characteristic parameters of laser heating system are specified. The mathematical model of the heating process is based on the heat equation with effective heat conductivity. Such an analysis allows to estimate effective thermal diffusivity and thermal conductance including Kapitza conductance. For multi-layer nano-films Kapitza conductance can be estimated as its contribution to effective conductance is significant.

1. Introduction

Transverse heat transfer in multilayer nanostructures can be described by the Fourier law with an effective thermal conductivity [1]. This value takes into account the distribution of heat in alternating layers and interface thermal conductance (Kapitza conductance) [2–4]. In the case of small thicknesses of the layers the Kapitza conductance is comparable with thermal conductance of the layer, and it may be a determining factor in some cases. Contribution of Kapitza conductance can be estimated from the measured values of the effective thermal conductivity at various layer thicknesses.

In the present work we consider some features of pulse heating method to study the main regularities of changes in the temperature of thin films, taking into account the heat exchange with the surrounding space. Such a heating can be realized by a single pulse (flash method) [5] and its modifications [6]. They can be a series of repetitive pulses or a frequency modulated heating [7]. At relatively high temperatures, a series of pulses (or modulated radiation) potentially can achieve higher sensitivity. The characteristic radiation parameters are specified.

2. Theoretical background

In the pulse regime (flash method), temporal evolution of the temperatures of the front and back sides of the film are registered by high-resolution sensors. Typical time moments of the temperature time dependence can be considered with the result of the solution of the heat conduction equation. From this comparison the effective heat conductivity can be obtained as the warm-up time is connected with thermal diffusivity
\[ a = \frac{\lambda}{\rho C}, \]  

(1)

where \( \lambda \) is effective heat conductivity, \( \rho \) is averaged density of the film, \( C \) is specific heat.

According to the developed calculation procedure [1], the effective heat conductivity is

\[ \lambda = \delta \left[ \sum \frac{\delta_i}{\lambda_i} + \sum \sigma_i^{-1} \right]^{-1}, \]

(2)

where \( \delta \) is the total thickness of the multilayer film; \( \delta_i, \lambda_i \) and \( \sigma_i \) are thickness of layer, heat conductivity of layer and Kapitza conductance of interface, respectively.

For the case of very thin layers the contribution of Kapitza conductance can be comparable with thermal conductance of the layer or higher, so one can estimate \( \sigma \sim \delta / (\lambda N) \), where \( N \) is the number of interfaces.

Under planar heat wave approximation, the mathematical model is based on the heat equation

\[ \rho C \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} \]

with non-steady boundary conditions

\[ -\lambda \frac{\partial T}{\partial x} = q_0 \varphi(t) - \alpha_1 (T - T_0) \quad \text{at} \quad x = 0 \quad (\text{front side}), \]

(4)

\[ -\lambda \frac{\partial T}{\partial x} = \alpha_2 (T - T_0) \quad \text{at} \quad x = \delta \quad (\text{back side}). \]

(5)

Here \( T = T(x, t) \) is the temperature, \( T_0 \) is the temperature of the environment, \( t \) is the time, \( x \) is transversal coordinate, \( q_0 \) is typical heat flux on front side of the film, \( \varphi(t) \) is the dimensionless heating time profile function, \( \alpha_1 \) is heat transfer coefficient for the front side, \( \alpha_2 \) is heat transfer coefficient for the back side (\( \alpha_1 \) and \( \alpha_2 \) includes radiation and, if needed, convective heat transfer).

Introduce dimensionless variables:

\[ t \rightarrow \frac{t}{\tau_1}, \quad x \rightarrow \frac{x}{\delta}, \quad T \rightarrow \frac{T - T_0}{\Delta T}, \]

where \( \tau_1 \) is the heat pulse duration, \( \Delta T \) is typical temperature variation.

Typical values of heat flux and temperature variation are the following:

\[ q_1 = \frac{Q}{S\tau_1}, \]

(6)

\[ \Delta T = \frac{Q}{S\delta\rho C}, \]

(7)

where \( Q \) is the energy of the pulse, \( S \) is the heat spot area (the area of the laser beam cross section approximately).

In dimensionless variables, the equations (3)–(5) take the following form:
\[
\frac{\partial T}{\partial t} = Fo \frac{\partial^2 T}{\partial x^2},
\]
(8)

\[-\frac{\partial T}{\partial x} = \frac{1}{Fo} \varphi(t) - Bi_1 T \quad \text{at } x = 0
\]
(9)

\[-\frac{\partial T}{\partial x} = Bi_2 T \quad \text{at } x = 1
\]
(10)

Here \( Fo = \frac{\lambda \tau_1}{\rho C \delta^2} = \frac{\alpha \delta}{\delta^2} \) is Fourier number, \( Bi_1 = \frac{\alpha_1 \delta}{\lambda} \) is the front side Biot number, \( Bi_2 = \frac{\alpha_2 \delta}{\lambda} \) is the back side Biot number.

Let’s estimate typical parameters of the heating laser system required to study effective heat conductivity of the film with thickness \( \delta \sim 100 \text{ nm} \). Assume the following parameters of the film material: \( \rho \sim 5 \times 10^{3} \text{ kg/m}^3, C \sim 300 \text{ J/(kg-K)}, \lambda \sim 50 \text{ W/(m-K)}, a \sim 3 \times 10^{-3} \text{ m}^2/\text{s} \). Heat spot area estimated as \( S \sim 10^{-6} \text{ m}^2 \), temperature variation \( \Delta T \sim 10 \text{ K} \). Under such a condition we obtain the heating energy \( Q \sim 10^{-7} \text{ J} \). Relaxation time for the material is about \( 10^{-11} \text{ s} \). So, the pulse time \( \tau_1 > 10^{-10} \text{ s} \) is needed. The corresponding power in pulse is \( Q/\tau_1 < 1 \text{ kW} \). The warm-up time (the time required for the back surface to reach half of the maximum temperature rise) is \( [5] \tau_{1/2} \sim (0.1/Fo)\tau_1 \). At \( Fo \sim 0.1 \) this value is \( \tau_{1/2} > 10^{-10} \text{ s} \).

3. Results and conclusions

We consider case of square pulse form, which is appropriate for the analysis of the effect of Biot numbers. In figure 1, time dependences of the temperatures of the front and back sides of the film surfaces are presented for the case with no heat transfer to the environment (\( Bi_1 = Bi_2 = 0 \)). The effect of heat transfer (the influence of \( Bi_1 \) and \( Bi_2 \) values) is shown in figure 2. One can see that maximal temperatures decreases with finite \( Bi_1 \) and \( Bi_2 \). So, the heating half-time \( \tau_{1/2} \) is changing, too.

**Figure 1.** Changing the temperature of the front side (1) and back side (2) with time at \( Bi_1 = Bi_2 = 0 \): \( a - Fo = 0.5, b - Fo = 0.25 \).
Figure 2. Changing the temperature of the front side (1) and back side (2) with time at $Fo = 0.1$: 
$a - Bi_1 = 0, Bi_2 = 0$; $b - Bi_1 = 1, Bi_2 = 0$; $c - Bi_1 = 0, Bi_2 = 1$; $d - Bi_1 = 1, Bi_2 = 1$.

Figure 3. The influence of Biot numbers on half temperature rise time ($a$) and maximal temperature of back side ($b$): $1 - Fo = 0.1, Bi_1 = \text{var}, Bi_2 = 0$; $2 - Fo = 0.5, Bi_1 = \text{var}, Bi_2 = 0$; $3 - Fo = 0.1, Bi_1 = Bi_2$; $4 - Fo = 0.5, Bi_1 = Bi_2$. 
Figure 3 shows the influence of Biot numbers on half temperature rise time $\tau_{1/2}$ and maximal temperature of back side $T_{2m}$. In the first case, only the Bio number changes for the front side of the film, the Bio number for the back side is taken to be zero (heat-insulated surface). In the second case, the same heat transfer is assumed for both sides of the film, that is, the Bio numbers are assumed to be equal for both sides.

We analyzed the effect of heat transfer when a thin film was heated to measure its thermal diffusivity by the flash method. The requirements to the heating system were also formulated depending on the thickness of the film. The results obtained improve the accuracy of the measurement procedure.

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